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The Effect of Methanol on the Mobilization of Tetrachloroethylene in a Water-Saturated Soil Column

A thesis submitted in partial satisfaction of the requirements for the degree Master of Science in Civil Engineering

by

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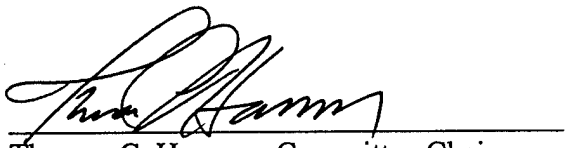

Thomas C. Harmon, Committee Chair

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Dedication

I would like to dedicate this thesis to my wife May for her unconditional support of my academic pursuit and military career. A special thanks to my parents Ron and Della, and my brother Scott, for all their help. Finally, to my son Brandon, who was born during the preparation of my thesis, for helping me maintain my sense of humor!

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ABSTRACT OF THE THESIS

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Professor Thomas C. Harmon, Chair

The contamination of surface waters and groundwater by chlorinated solvents continues to be a major environmental issue. Today, the challenge to environmental engineers is not necessarily which remediation technique to use, but how to enhance the remediation technique in order to accelerate the clean-up process.

The "pump-and-treat" method for remediating organic contaminants is experimenting with the use of chemical additives to increase the efficiency rate of subsurface contaminant removal. Because of their favorable chemical properties, alcohols such as methanol are often used in conjunction with water to flush a contaminated area, and subsequently pump it to the surface for treatment. For this study,

the objectives were: (1) to reconfirm the impact of a cosolvent, such as methanol, on the observed retardation of nonpolar organic solute (tetrachloroethylene, PCE) transport in a water-saturated porous medium; and, (2) to provide evidence that ineffective mixing of two inhomogeneous fluids, such as methanol and water, can negatively impact the desired cosolvent effect.

For the one-dimensional laboratory column at the flowrate tested (0.745 mL/min), methanol failed to produce the hypothesized cosolvent effect. The degree of retardation of PCE did not decrease log-linearly, but instead showed no significant difference with increasing methanol fraction. Therefore, the column system, under the conditions used in this study, may have been subject to the ineffective fluid mixing potentially associated with cosolvent-water systems. However, breakthrough behavior for methanol was generally symmetric and failed to exhibit any signs of ineffective mixing. The nature of these results underscores the complexity of the problem of mixing of inhomogeneous fluids.

Chapter 1. Introduction

Chlorinated solvents, used as cleaning agents in a vast array of industries, from dry cleaning to aerospace, are known or suspected as either carcinogens or mutagens. The frequent industrial use of these chemicals, such as tetrachloroethylene (PCE), trichloroethane (TCA), and trichloroethylene (TCE), has led to widespread contamination of soil and groundwater. Because of the high volatility of these organic compounds, their concentrations in surface waters, which are only a few micrograms per liter, is not a water quality issue. However, it is in the groundwater where the concentrations of chlorinated solvents will be thousands of times higher since the contaminants cannot volatilize, and hence will tend to remain in water or sorb to soil. Most frequently, the corrective action for subsurface contamination is to flush the contaminated area with water and subsequently pump it to the surface for treatment. This conventional "pump-and-treat" (Mackay and Cherry, 1989) strategy is effective for removal of a majority of the contaminant. Unfortunately, the remaining contaminant is still, most often, well above prescribed limits.

The remaining contamination is often due to nonaqueous phase liquids (NAPLs) in the subsurface. NAPLs are immiscible in water and can have densities that are either greater than water or less than water. When a NAPL has a density greater than water, it is commonly referred to as a dense nonaqueous phase liquid (DNAPL). Conversely, if the NAPL's density is less than water, it is commonly referred to as a light nonaqueous phase liquid (LNAPL). Examples of DNAPLs include chlorinated solvents such as trichloroethylene. Some examples of LNAPLs include gasoline, petroleum oil, and diesel fuel. The continued presence of NAPLs in the subsurface poses a major clean-up problem. It is critical to locate and remove any NAPLs from a hazardous waste site because NAPLs provide a long-term source of pollution due to their low solubilities.

Because of the limitations of the "pump-and-treat" method for remediating NAPL organic contaminants, alternative remediation techniques such as bioremediation and chemical additives are being considered.

1.1 Bioremediation

Bioremediation is the use of microorganisms to degrade subsurface contaminants. The microorganisms, generally bacteria, convert harmful chemical compounds to less harmful chemical compounds in order to effect remediation of a contaminated site. To survive, the microbes require: a carbon supply, an energy supply, and nutrients. The types and amounts of carbon, energy, and nutrients, are part of the overall design of the remediation system. Therefore, a detailed understanding and control of the site hydrogeology is required to implement an efficient remediation effort. Contaminant factors, such as: solubility, volatility, viscosity, and toxicity; and soil conditions, such as: permeability, soil type, depth to groundwater, mineral content, oxidation/reduction potential, and pH; may have a profound affect on the general remediation design.

The key to successful bioremediation is engineering the system such that all the microbe requirements can combine in the subsurface. However, engineering the system is not as simple as one might expect. The geologic medium for remediation must be permeable enough to allow the introduction of energy and nutrients. Many intraparticle pores are too narrow to allow microbe access. If the microbes cannot reach the zone of contamination, the remediation effort will fail. Another limitation to bioremediation is that it is difficult to biostimulate immobile zones. Most often, the contaminant must diffuse out to the biostimulated zone before bioremediation can occur. Finally, bioremediation is still in the developmental stage and there are few documented cases of using bioremediation in the saturated zone.

1.2 Chemical Additives

Enhanced remediation techniques using chemical additives are being introduced to increase the efficiency rate of contaminant removal from the subsurface (Palmer *et al*, 1992; Augustijn *et al*, 1994). In-situ solvent flushing involves injecting a mixed solvent into the subsurface of a site contaminated with organic chemicals. Surfactants, alcohols, or mixtures of these chemicals are often used as the solvent (Imhoff, 1995). When the solvent is in sufficient quantities relative to water, it is often referred to as a water-miscible organic *cosolvent*. Miscibility describes a compound's ability to mix in any ratio with water without separation into two phases, while immiscibility means a compound is unable to mix with water. Because of their favorable chemical properties, alcohols, such as methanol, have been investigated as potential cosolvents.

1.3 Thesis Overview

The objective of this thesis study is to test the ability of methanol as an effective cosolvent. Through a series of experiments, this research will investigate: the transport and dissolution of methanol in a water-saturated porous medium and, the effects of methanol on the mobilization of PCE. The hypothesis of this study is that methanol will decrease the retardation factor of PCE in a porous medium, thereby confirming the impact of cosolvents on remediating hazardous organic compounds.

In Chapter Two, background material relating to organic contaminants will be presented. Chapter Three will delve into the theory of cosolvency and subsurface remediation. In Chapter Four, the research objectives and approach for this thesis will be outlined. Chapter Five will detail the experimental methods used, and Chapter Six will

highlight the results. Finally, in Chapter Seven, a summary of the findings, and the conclusions reached in this study, will be presented.

Chapter 2. Background

Before reviewing the underlying theory of cosolvency, it is instructive to examine background material relating to organic contaminants and their properties, properties affecting the transport of a NAPL-based solute, and physical properties affecting the fate and transport of organic chemicals in groundwater.

2.1 Organic Contaminants and their Properties

Organic contaminants, such as TCE and PCE, are just two of the myriad of chlorinated solvents found in the subsurface. The extent to which these solvents contaminate the subsurface depends, in part, on the properties of the organic contaminants. Polarity refers to the extent of the dipole moment in a molecule. Hydrophobicity is the tendency of organic compounds dissolved in groundwater to adsorb onto solid surfaces. Less polar molecules are more hydrophobic. Solubility refers to the concentration of a species in a saturated aqueous solution. TCE and PCE have low solubilities due to their lack of polarity; hence, they are commonly referred to as hydrophobic contaminants.

2.2 Properties Affecting Transport of a NAPL-based Solute

Several key properties affect the transport of a NAPL-based solute. Solubility plays a major role. Another important property is sorption. Sorption is the term used to describe adsorption and/or absorption when independent determination of the processes is impossible. Adsorption is the net accumulation of a solute at the solid-liquid interface; while absorption occurs when a solute is transferred from one phase (i.e., water) to another, such as soil or organic matter.

2.3 *Physical Processes Affecting Fate and Transport of Organic Chemicals in Groundwater*

Organic contaminants may enter the subsurface by spills, leaks, or intentional disposal. In the saturated zone, these organic chemicals will either dissolve in the groundwater or will remain immiscible with groundwater in the form of NAPLs. A review of the physical processes that most strongly influence this phenomena will be presented to assist in the understanding of organic contaminant transport and distribution in the saturated zone.

2.3.1 The Advection-Dispersion Equation

Transport phenomena in the saturated zone is governed by the *Advection-Dispersion* equation (e.g., Freeze and Cherry, 1979):

$$\underset{(1)}{\frac{\partial C}{\partial t}} = \underset{(2)}{\frac{\partial}{\partial x}\left(D_{HD}\frac{\partial C}{\partial x}\right)} - \underset{(3)}{\frac{\partial}{\partial x}\left(v_X C\right)} \qquad (2\text{-}1)$$

where D_{HD} = hydrodynamic dispersion coefficient [L^2/T]
v_X = the average pore water velocity [L/T]
t = time [T]
x = distance [L]
C = solution concentration [M/L^3]

The first term (1) is the net accumulation. Term (2) represents the transport due to dispersion and term (3) represents the transport due to advection.

A more complete modeling of the transport of the solute in the aquifer would consider the immobile zones in each molecule of porous media. To account for this property of the media the concept of *retardation* will be introduced in Section 2.3.4.

2.3.2 Advection

Saturated-zone transport of dissolved contaminants is due primarily to advection. Advection is the process by which a solute is transported by the movement of the fluid itself (i.e., groundwater flow). The flow of groundwater is driven according to Darcy's Law. It is important to be able to estimate the rate at which groundwater is moving through an aquifer. This rate, the Darcy velocity, can be found by solving for the velocity using Darcy's Law (2-2).

$$Q = - KA \frac{\partial h}{\partial L} \qquad (2\text{-}2)$$

where Q = flow rate [L^3/T]
K = hydraulic conductivity or coefficient of permeability [L/T]
A = cross-sectional area [L^2]
$\frac{\partial h}{\partial L}$ = hydraulic gradient

The Darcy velocity is not the actual groundwater velocity because the cross-sectional area, given by A in (2-2), of an aquifer is made up of solids. The actual cross-sectional area is much smaller, and hence, the actual groundwater velocity is considerably faster than the Darcy velocity.

Groundwater will flow from points of high piezometric head to points of low piezometric head. The difference in water elevation and pressure head between points determines the hydraulic gradient which drives the flow of groundwater. In gentle topography and under unconfined conditions, the gradient normally follows the topography, and the groundwater flow rate can be estimated within a factor of 10 (Roberts *et al*, 1986). However, several factors, such as a porous media's hydraulic conductivity, can make the determination of the groundwater flow rate quite difficult to

estimate. Hydraulic conductivity is a measure of the ability of a porous media to transmit a fluid (i.e., water) and is dependent on the properties of the porous media and the fluid.

A subsurface porous media found in nature is generally *heterogeneous*; that is, the hydraulic conductivity varies from place to place. The porous media is considered to be *homogeneous* when the hydraulic conductivity is the same throughout. Sometimes hydraulic conductivities are a function of the flow direction. Generally, hydraulic conductivities are higher in the horizontal direction than in the vertical direction (Freeze and Cherry, 1979). Aquifers that have the same hydraulic conductivity in any flow direction are called *isotropic*, while those aquifers in which the conductivities varies according to direction are called *anisotropic*. Because *homogeneous* and *isotropic* aquifers are rarely found in nature, one must collect empirical measurements to obtain reasonably accurate estimates of the groundwater velocity in a flow field.

For one-dimensional soil column experiments, such as the one used for this study, a homogeneous and isotropic aquifer can be simulated. Because a pore water velocity is typically known for this type of system, the flow equation (2-2) is not employed. A one-dimensional, homogeneous and isotropic porous medium will limit variations from occurring. However, the limitation of this lab system is readily apparent in that it is not representative of an actual environmental system.

2.3.3 Dispersion

Dispersion is the tendency of a solute to spread during transport. The two main causes of dispersion are mechanical mixing and molecular diffusion (Freeze and Cherry, 1979). Mechanical mixing is mixing due to velocity gradients. The factors which affect the degree of mechanical mixing include: different sized pore channels within the porous media, variations in pore geometry (tortuosity), and fluctuations in the local flow

velocities relative to the mean flow direction. Molecular diffusion is the net flux of a solute from a zone of high concentration to a zone of low concentration. Dispersion results in the dilution of contaminant pulses and the attenuation of concentration peaks. Therefore, the maximum concentrations diminish with increasing distance from the source (Mackay *et al*, 1985).

Dispersion can occur longitudinally, in the principal direction of flow; or transversely, perpendicular to the principal direction of flow. The hydrodynamic dispersion coefficient is a tensor (Bear, 1972):

$$D = \alpha_L D^1 + \alpha_T D^2 + D^* \qquad (2\text{-}3)$$

where D = hydrodynamic dispersion coefficient [L^2/T]
D^* = coefficient of molecular diffusion, which is generally ignored [L^2/T]
α_L = longitudinal dispersivity of the porous medium [L]
α_T = transverse dispersivity of the porous medium [L]

For the one-dimensional case,

$$D^1 = v \text{ and } D^2 = 0 \quad \text{where } v = \text{Darcy velocity [L/T]}$$

Therefore,

$$D = \alpha_L (v) \qquad (2\text{-}4)$$

Despite the practical importance of the dispersion process, there is currently no method to confidently predict the magnitude of dispersion for a previously unstudied field situation. For simple hydrogeological systems, the spreading is believed to be proportional to the flow rate. For more complex systems, the dispersivity appears to

depend on the structure of the geologic medium such that it varies with the distance traversed (Mackay *et al*, 1985).

2.3.4 Retardation

Retardation is the apparent slowing of contaminant transport relative to groundwater flow due to sorption. The higher the fraction of the contaminant sorbed, the more retarded is its transport (Mackay *et al*, 1985).

Sorption of halogenated chemicals to soils is a nonspecific combination of two factors. The first factor is related to hydrophobicity. In essence, the molecules are "squeezed out" of the water and deposited on the soil surfaces due to their hydrophobicity (e.g., Curtis *et al*, 1986). The second factor affecting sorption is the fraction of solid organic matter in the aquifer solids, known as organic carbon content. Attempts have been made to correlate organic contaminant sorption with soil organic matter and a chemical property of the contaminant such as the octanol-water partition coefficient (Karickhoff *et al*, 1979). The assumption is that all sorption is due to organic matter implying the amount of sorption is proportional to the amount of organic matter.

If a solute does not sorb to the porous medium, it will move at a velocity equal to the groundwater velocity and, by definition, has a retardation factor equal to one. However, if the solute does sorb to the soil, it will move at a velocity equal to the groundwater velocity divided by a retardation factor, R:

$$R = 1 + \frac{\rho K_d}{\theta} \qquad (2\text{-}5)$$

where ρ = soil bulk density $[M_s/L^3]$
θ = soil porosity [-]
K_d = equilibrium distribution coefficient $[L^3/M_s]$

The equilibrium distribution coefficient is a function of the soil and the chemical type. Numerous attempts have been made aimed at correlating K_d with chemical properties, such as solubility or octanol-water partitioning coefficient (Karickhoff, 1979; Chiou *et al*, 1983; Curtis *et al*, 1986). These attempts assume that the sorption process is attributed solely to the soils organic carbon fraction. However, other studies (e.g., Ball and Roberts, 1991a) have shown that for soils characterized by low organic carbon contents (i.e., about 0.1% or less w/w), mineral surfaces play a significant role. In any case, the published correlations are best used for a first approximation, and more accurate K_d estimates must be determined experimentally.

2.4 Groundwater Remediation

Contaminated groundwater can contain an abundance of organic chemicals. Due to the low solubility of some of these chemicals, large dilute plumes of contaminant typically appear and propagate through the saturated zone. The most common method of treatment for a contaminated aquifer is a pump-and-treat system. The contaminated groundwater is extracted via a withdrawal well and treated at the surface through a filtration process such as granular activated carbon.

2.4.1 Effect of Sorption on Remediation

In an aquifer, one might expect a contaminant to move at the same speed as the groundwater; however, this is not necessarily the case. Some contaminants are sorbed onto the soil particles thereby reducing the overall solute flow rate relative to that of the groundwater itself. The solute is retarded by a factor R called the retardation factor. For a successful remediation, R pore volumes must be extracted under ideal conditions (assuming the local equilibrium assumption (LEA) applies: no immobile zones and

instantaneous equilibrium is achieved between the water and solid phases). Thus, reducing sorption (or R) would expedite the remediation process.

2.4.2 Nonequilibrium Sorption

Equilibrium sorption models such as LEA assume that the mass transfer rate is fast relative to the flow rate so that equilibrium can be reached. If this is not the case and equilibrium is not attained, a nonequilibrium sorption model is more appropriate. Unfortunately, a kinetic model causes complications at two scales. At the particle scale, mass transfer resistances like intraparticle diffusion can markedly decrease the rate of contaminant release from a sorption site thereby increasing remediation times (e.g., Ball and Roberts, 1991a; Harmon and Roberts, 1994). At the layer scale, an increase in the degree of hydraulic conductivity due to heterogeneity (larger scale immobile or low flow zones) can be a dominant factor in causing remediation times to increase (Rabideau and Miller, 1994; Kong and Harmon, 1996).

2.4.3 Effect of Cosolvents on Retardation

At the particle scale, complications caused by nonequilibrium sorption can be mitigated by the use of cosolvents (Brusseau *et al*, 1991). Cosolvents can lower retardation factors and increase mass transfer rates. This thesis will examine the capacity of a cosolvent to lower the retardation factor of PCE. Before examining the Research Objectives and Approach, Cosolvency Theory and Subsurface Remediation will be reviewed in detail in the next chapter.

Chapter 3. Cosolvency Theory and Subsurface Remediation

The idea of using cosolvents to accelerate the remediation of soils and groundwater has recently been considered for field testing (Augustijn *et al*, 1994). Although a relatively new remediation technique for soil and groundwater, the technology was actually developed in the petroleum industry. The mechanisms involved in cosolvent flooding for enhanced oil or nonaqueous phase liquid (NAPL) recovery have been discussed in several reviews (Reed *et al*, 1977; Larson *et al*, 1982; Lake, 1983; Imhoff *et al*, 1995). Other studies have indicated that the use of cosolvents will reduce the retardation factor substantially, thereby vastly reducing the remediation times (Yalkowsky *et al*, 1981; Rao *et al*, 1985; & Nkedi-Kizza *et al*, 1989).

3.1 Methanol as a Cosolvent

Methanol is a colorless, polar chemical that is miscible with water. Today, methanol has many industrial and consumer uses. Approximately 70% of the methanol produced worldwide is used in chemical syntheses (Ullman, 1990). The most readily apparent use of methanol is as an energy source. The oil crisis in the early 1970's set in motion the need to find alternative sources of fuel. Coupled with the added emphasis on air quality, methanol and methanol-petroleum fuel mixtures were a good solution. As the 21st century approaches, the use of methanol is increasing. Because of methanol's low freezing point and miscibility with water, it is sometimes used in refrigeration systems. Moreover, it is used as an anti-freeze or an absorption agent in gas scrubbers.

Methanol is an excellent choice for a cosolvent. Recent studies (e.g., Imhoff *et al*, 1995) cite methanol's advantages: (1) it is relatively inexpensive; (2) once diluted to low concentrations in groundwater, it is readily biodegradable; and (3) it is representative of a class of alcohols that do not significantly partition into denser than water nonaqueous

phase liquids (DNAPLS), and thus will not enhance downward DNAPL migration by reducing the interfacial surface tension of the DNAPL residual ganglia.

3.2 Cosolvent Theory

The idea of including other organic molecules in water to affect the solubility of organic contaminant in a solution is the basis behind the theory of cosolvency. When the organic molecules are present in relatively large quantities ($\cong >$ 10% volume/volume), they act as solvent molecules themselves and partially surround the solute of interest, approximately in proportion to their volume fraction in the solution (Yalkowsky *et al*, 1976). If the organic molecules are not present in these quantities, the effect on solubility ranges from *no effect* (for < 0.001 v/v) to a *slight effect* (for > 0.001 but < 0.10).

Yalkowsky *et al* (1976) postulated that the excess free energy of solution of a solute in a water organic cosolvent mixture should be a linear combination of the solute's excess free energies of solution in each solvent alone. Part of the organic solute is dissolved in water and the remainder of the organic solute is dissolved in the organic cosolvent. By solving for the excess free energy of solution in pure water and the excess free energy of solution in the cosolvent, and by substitution, Yalkowsky *et al* (1976) showed mathematically that the log solubility of a solute increased linearly as the fraction of cosolvent in the solution mixture increased. This result was well supported by experimental observations conducted by Yalkowsky *et al* (1976) using a series of aromatic hydrocarbons.

3.3 Cosolvent (Methanol) Effects

A recent study (Imhoff *et al*, 1995) investigated the following topics: (1) the effect of methanol on various system parameters; (2) the influence of methanol on phase

partitioning; and, (3) the effect of methanol on PCE mobilization and rate of PCE dissolution. Conclusions were made after conducting a series of batch-contacting and generator column experiments.

3.3.1 Physical and Chemical Properties of PCE

The effect of methanol on various physical and chemical properties of PCE were determined for a select number of methanol/water volumetric fractions (0%, 20%, 40%, and 60% methanol by volume). The 60% methanol by volume results demonstrated that methanol significantly affected: the viscosity of the aqueous phase, the interfacial tension between the aqueous phase and PCE, the molecular diffusion coefficient of PCE, and most markedly, the PCE solubility. As their study (Imhoff *et al*, 1995) pointed out, an increased molecular diffusion coefficient and an increased solubility resulted in a faster remediation time.

3.3.2 Mobilization of PCE

Three column experiments were conducted to examine the effect of various methanol/water mixtures on the mobilization of trapped PCE ganglia (Imhoff *et al*, 1995). Although column experiments one and three resulted in no measurable PCE mobilization, experiment two demonstrated PCE mobility. The injection of a 60% methanol/water mixture into the column increased the aqueous phase viscosity, decreased the nonaqueous-aqueous phase interfacial tension, and increased the density difference between the nonaqueous and aqueous phases. It was readily apparent in the analysis of experiment two that the flushing of the column with the methanol cosolvent may have enhanced the downward migration (mobilization) of DNAPL ganglia.

3.3.3 Dissolution and Mass Transfer Rate Coefficient

Imhoff *et al* (1995) demonstrated that various methanol/water mixtures had an impact on the rate of PCE dissolution and the solubility limit of PCE in the aqueous phase. The change in the mass transfer rate coefficient with varying methanol fraction was due to the corresponding change in aqueous phase viscosity. When plotting the maximum potential mass flux versus the methanol fraction, the maximum potential mass flux was shown to increase by a factor of 30 as the methanol/water fraction increased from 0% to 60%. The improvement in the mass flux was attributed to the increase in aqueous phase PCE solubility.

3.3.4 Related Research

There are several publications on the effective use of cosolvents for enhanced in situ remediation. The major conclusions from these are briefly summarized in this section.

Nkedi-Kizza et al (1985) presented data in their study that clearly demonstrated the validity of the solvophobic approach for predicting the sorption of hydrophobic organic chemicals (HOC's) from binary solvent mixtures. They concluded that for each sorbate, the sorption coefficient decreased log linearly as the fraction of organic cosolvent increased.

Fu et al (1986) studied the hydrophobic sorptive behavior of four aromatic solutes onto three different soils with solvent/water mixtures. For a polar solvent, sorption decreased semi-logrithmically with an increase in volume fraction of solvent in the aqueous phase. This may have been the result of the solvent/water mixture swelling the organic carbon associated with the soil and thereby increasing solute accessibility to

organic matter. The conclusion of the study was that the more hydrophobic the solute, the greater the effect of solvent in solvent/water mixtures on solute solubility enhancement, and hence the less the tendency to sorb onto soil. Thus, the results of this investigation were particularly significant for those aromatic solutes exhibiting the lowest aqueous phase solubility.

Rao et al (1990) demonstrated that the presence of a completely miscible organic solvent (CMOS) increases the partially MOS solubility which in turn, is reflected in increased solubility and decreased sorption of hydrophobic organic chemicals (HOC's). Further, with increased volume fraction of a CMOS in a binary mixed solvent, HOC solubility increased and sorption decreased, essentially in a log-linear matter. They concluded that an increase in HOC solubility in the presence of cosolvents was reflected by decreased sorption by soils and increased mobility of HOC's.

Augustijn et al (1994) demonstrated in laboratory miscible displacement experiments that the smaller the retardation factor in water and the higher the cosolvent fraction, the faster the contaminant was recovered by solvent flushing. In addition, the presence of non-equilibrium conditions, soil heterogeneity, and the type of cosolvent influenced the time required to recover the contaminant. Augustijn *et al* found that solvent flushing was appropriate for more hydrophobic chemicals. Experimental data and model simulations showed that with increasing cosolvent content, the contaminant eluted at higher concentrations, thus improving the contaminant recovery efficiency. The conclusion of the study was that high cosolvent fractions were most effective for the elution of contaminants. The recovery efficiency was expected to decrease under non-equilibrium conditions and in a heterogeneous soil. The type of cosolvent and composition of the solvent mixture are design parameters that can be used to optimize the recovery efficiency.

Harmon et al (1994) focused on two aspects of methanol's behavior in the subsurface environment: (1) the mixing and dissolution; and, (2) the mobilization of sorbing organic contaminants. The studies were carried out in batch and column systems composed of a well-characterized sand fraction. All systems were water-saturated. The study examined: the impact of methanol on the sorption of the hydrophobic contaminant, benzene; the transport of methanol and benzene as solutes; the mixing behavior of methanol in a water-saturated soil column; and the impact of methanol mobilizing benzene in a water-saturated soil column. The results of the experiments showed that the retardation factor of benzene (i.e., sorption) decreased with increasing methanol fraction. However, at higher methanol fractions (>20%), there was an apparent increase in the retardation factor. They attributed the increase in retardation to the density difference between water and methanol. The major conclusions generated by the study were: (1) methanol reduces the equilibrium transport parameter (confirming results from previous studies); and (2) accurate modeling of the mixing of pure methanol with water in porous media requires addressing the water-methanol density differences.

3.3.5 The Mixing of Miscible, Inhomogeneous Fluids in the Subsurface

A major finding of the Harmon *et al* study (1994) was that there was a relatively poor understanding of the dynamics of mixing of miscible, inhomogeneous fluids in the subsurface environment. They found that the differences between methanol and water (i.e., density and viscosity) imply that the displacement of one fluid by the other will defy conventional flow and transport modeling approaches, which treat density and viscosity as constants. Currently, research is under way by Harmon *et al* (1996) to illustrate the dynamics of mixing and transport of miscible, inhomogeneous fluids in a porous medium

in hopes of increasing the understanding of, and design capabilities for, chemically enhanced remediation.

3.4 Thesis Objectives

The study by Harmon *et al* (1994) is the basis for this thesis. The impact of methanol as a cosolvent will be further investigated; in this case, on the nonpolar organic solute, PCE. Furthermore, this study will investigate the mixing dynamics of miscible, inhomogeneous fluids (methanol and water) in the context of soil and groundwater remediation strategies.

Chapter 4. Research Objectives and Approach

As with the previous study (Harmon *et al*, 1994), the research approach for this masters thesis focuses on the study of a one dimensional, single aquifer solid type. However, the organic contaminant to be used in conjunction with methanol is PCE instead of benzene.

4.1 Research Objectives

The objectives of this study were two-fold:

(1) To reconfirm the impact of a cosolvent (i.e., methanol) on the observed retardation of nonpolar organic solute PCE transport in a water-saturated porous medium.

(2) To provide evidence that ineffective mixing of two inhomogeneous fluids (i.e., methanol and water) can negatively impact the desired cosolvent effect.

4.2 Experimental Approach

The porous media used in this study is Borden sand (-40+60 U.S. Standard mesh size, mean particle diameter = 0.33 mm). The experiments performed in the study were:

(1) Tracer Experiments- Breakthrough curves of trace amounts of ^{14}C-labeled methanol/PCE in water to examine their transport behavior.

(2) Methanol Displacement Experiments- A series of breakthrough curves for examining the transport of various methanol fractions through the sand column.

(3) PCE Mobilization Experiments- A series of breakthrough curves to observe methanol mobilizing PCE in a saturated soil column.

4.3 Theoretical Approach

The results obtained from these experiments were modeled using available analytical solutions to the advection-dispersion equation. In the tracer experiments, trace amounts of MeOH in water were run through the column. The goal was to generate breakthrough curves which would provide a basis of comparison for the methanol displacement experiments and PCE mobilization experiments.

In the next set of experiments, the goal was to determine the advection and dispersion characteristics of methanol as a solute and as a cosolvent. Five individual tests were conducted. The methanol fractions used for each of the test pulses were 1%, 5%, 10%, 20%, and 50%. Using the soil-column lab set-up discussed in Chapter Five, forty experimental data points were measured in each test and used to characterize a specific methanol breakthrough curve. A least-squares fitting program, CFITM, (van Genuchten, 1981) was used to find the Peclet number for each data set assuming a retardation value of one. CFITM is a FORTRAN program capable of solving the nondimensional form of the Linear equilibrium adsorption (LEA) model (LEA model discussed in Section 5.1). With a Peclet number for each methanol fraction, the stage would be set for the next set of column experiments.

In the final set of experiments, the goal was to determine how the different methanol fractions would affect the mobilization of PCE in the soil column. Using the same experimental set-up, forty experimental data points were measured for each methanol fraction. Using the Peclet number generated from the previous set of experiments, CFITM was used to fit the retardation factor. The fitted retardation factor would be an indication of methanol's ability to mobilize PCE.

Chapter 5. Modeling Approach and Experimental Methods

5.1 Modeling Approach

Transport of a nonsorbing solute in a one-dimensional water-saturated porous medium is governed by the advection/dispersion equation (e.g., Freeze and Cherry, 1979):

$$\frac{\partial C}{\partial t} = D_{HD}\frac{\partial^2 C}{\partial x^2} - v_X\frac{\partial C}{\partial x} \qquad (5\text{-}1)$$

where D_{HD} = hydrodynamic dispersion coefficient [L^2/T]
v_X = the average pore water velocity [L/T]
t = time [T]
x = distance [L]
C = aqueous concentration [M/L^3]

Equation (5-1) assumes steady-state flow and no interactions between the aqueous phase and the solid phase.

If chemical adsorption is considered, an additional term is needed to account for the interaction between the aqueous phase and the solid phase and the advection/ dispersion equation becomes:

$$\frac{\partial C}{\partial t} = D_{HD}\frac{\partial^2 C}{\partial x^2} - v_X\frac{\partial C}{\partial x} - \frac{\partial S}{\partial t} \qquad (5\text{-}2)$$

where S = adsorbed concentration [M/M].

Prior to the conception of the CFITM model, significant deviations were observed between the calculated and experimental effluent curves using equation (5-2). In an

attempt to account for these apparent differences, several models were introduced (for review, see Harmon *et al,* 1989). The increasing complexity with which the immobile zones were viewed (described by the S term) led to CFITM. (van Genuchten, 1981).

In his program CFITM, van Genuchten (1981) considers five conceptual models. Depending on the exact form of the transport model, the program allows up to five different parameters to be estimated simultaneously. The least-squares computer model fits these transport parameters to column effluent data. The five transport models are:

Model A: Linear equilibrium adsorption

Model B: Physical non-equilibrium

Model C: Physical non-equilibrium in the presence of anion exclusion

Model D: Two-site kinetic non-equilibrium adsorption

Model E: One-site kinetic non-equilibrium adsorption

The model used for this work is the Linear Equilibrium Adsorption Model (LEA). With the LEA model, the relationship between the aqueous concentration and the sorbed concentration is described by a linear isotherm:

$$S = K_d C \qquad (5\text{-}3)$$

where K_d is an empirical distribution coefficient [L^3/M_s]. Substitution of equation (5-3) into equation (5-2) yields the following transport equation:

$$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} \qquad (5\text{-}4)$$

where R is the retardation factor [-] equal to:

$$R = 1 + \frac{\rho K_d}{\theta} \qquad (5\text{-}5)$$

where ρ = soil bulk density [M_s/L^3]
θ = soil porosity [-]
K_d = empirical distribution coefficient [L^3/M_s]

The program requires input data for the following dimensionless variables in order to perform the analysis of the effluent data:

(1) Length (Z) = x/L L = length of porous media

(2) Concentration (C) = C/C_o C_o= influent concentration

(3) Pore volumes (T) = $v_x t/ L$

(4) Peclet Number (P) = $v_x L/ D_{HD}$

For the dimensionless parameter (4), the Peclet number is defined as the ratio of advective flux to dispersive flux. A high Peclet number means advection is dominating transport while a low Peclet number implies dispersion is dominating transport. Typical Peclet number values for natural flow in groundwater ranges from one to five; however, these values may be greater under pumping conditions (Mackay *et al*, 1985).

To use van Genuchten's model, one must input the Peclet number, the retardation factor, the length of the input (pulse), and the data points (in dimensionless form). The user can request the program to fit one, two or all three parameters (Peclet number, retardation factor, and length of input). The fitted parameters are obtained by means of a

least-squares fit of the appropriate analytical solution to column effluent data. By iteration, a fitted solution is obtained. The non-linear least squares analysis output gives the fitted parameter value and a 95% confidence interval of the results. Although relatively old (1981), van Genuchten's program is not obsolete. The program is versatile and can be dimensioned for up to 90 data points. The least-squares computer model provides a convenient, efficient, and accurate means of fitting various transport parameters to column effluent data (van Genuchten, 1981).

5.2 Model Boundary Conditions

Analytical solutions of equation (5-4) exist for several sets of initial and boundary conditions. In van Genuchten's study (1981) for the LEA model, the initial condition is:

$$C(x,0) = C_i \qquad (5\text{-}6)$$

Two different conditions can be applied to the upper boundary of the soil column (x = 0): a first-type, constant concentration boundary condition of the form:

$$C(0,t) = C_o \qquad (5\text{-}7)$$

or a second-type, constant flux boundary condition of the form:

$$\left(-D \frac{\partial C}{\partial x} + vc\right)\Big|_{x=0} = v\,C_o \qquad (5\text{-}8)$$

where C_o is the concentration of the input solution.

For the lower boundary, the following condition is applied:

$$\frac{\partial C}{\partial x}(\infty,t) = 0 \qquad (5\text{-}9)$$

This condition assumes the presence of a semi-infinite soil column. An alternative boundary condition, one that is frequently used for column displacement studies, is that of a zero concentration gradient at the lower end of the column:

$$\frac{\partial C}{\partial x}(L,t) = 0 \qquad (5\text{-}10)$$

where L is the column length.

In van Genuchten's study (1981), equations (5-9) and (5-10) are both used. However, only the solutions for a semi-infinite medium are included in the curve-fitting program. Because of the relatively small influence of the imposed mathematical boundary conditions, the solutions for a semi-infinite system provide close approximations for those applicable to a physically well-defined finite system, especially for not too short laboratory soil columns.

5.3 Experimental Methods

Each of the experiments summarized in Chapter 4.3 is described in detail in the following section.

5.3.1 One-Dimensional Column Set-up

The set-up of the soil column experiments is shown schematically in Figure 5-1. The controlled flow of methanol and water was driven through the soil column using a quarternary high performance liquid chromatography (HPLC) pump (Paramus, NJ) in

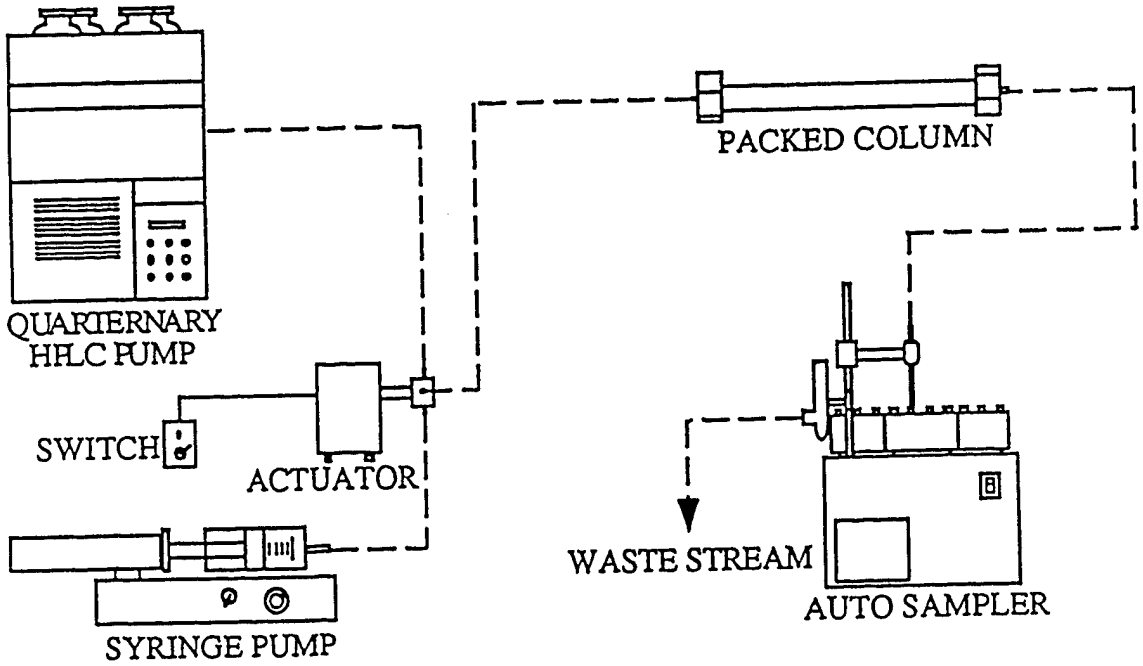

Figure 5-1. Schematic diagram of column study experimental set-up

order to deliver precise mixtures of methanol and water. In this study, a 25-cm steel column (2.06 cm inner diameter) was used, packed with -40+60 (U.S. Std. Mesh Size) Borden sand, which had been examined in particle characterization and organic contaminant sorption and desorption studies with PCE (Ball *et al*, 1990; Ball and Roberts, 1991a; 1991b; Harmon and Roberts, 1994). The Borden sand has: a mean grain diameter of 0.33 mm; a density of 2.71 g/cm^3; and an organic carbon content of 0.00023% (Ball *et al*, 1990). The porosity was approximately 0.35. The ^{14}C-labeled solute, either methanol or PCE, was injected via a gastight syringe mounted on a syringe pump (Sage Model 341B, Boston, MA). A three-way, electronically actuated valve (Valco, Houston, TX), which allowed precise switching between the HPLC pump and the syringe pump, was used for inputting the ^{14}C-labeled solute pulse. The data points for the effluent breakthrough curves were captured in a series of vials containing liquid scintillation cocktail fluid. All fittings were composed of glass, Teflon, and stainless steel to avoid interactions between the organic contaminants and the apparatus.

5.3.2 Analytical Methods

5.3.2.1 Liquid Scintillation Counting

Liquid scintillation vials typically contained 5 mL of liquid scintillation cocktail (Insta-gel, Packard Instrument Co., Downer's Grove, IL). The samples were counted with a Packard Tricarb Model 4530 scintillation counter (Packard Instrument Co.). All samples were counted two times for 20 minutes each. Measured counts per minute were converted to actual disintegrations per minute by the external standard method, with quenching efficiencies estimated by a channels ratio method incorporated into the system software. Quenching was less than 5% for all samples and in a spectral region where

quenching was relatively insensitive to changes in solution matrix. Each set of vials to be counted was accompanied by a blank sample (containing 5 mL of scintillation cocktail), used to subtract out background activity.

5.3.2.2 Gas Chromatography

Prior to each spiking session, the overall (labeled and non-labeled) concentration of the spiking solution was determined by comparison with standard solutions using gas chromatography. Samples of the spiking solution were prepared by extracting approximately 3 mL of the spiking solution with 0.5 mL pentane in 2 mL vials equipped with teflon-lined silicon septa and plastic screw-top caps (Alltech Assoc., Deerfield, IL). Samples and standards were also spiked with an internal standard (1-chloro, 2-bromopropane). The PCE and internal standard were extracted into the pentane during 30 minutes of agitation on a shaker table.

The gas chromatograph, a Hewlett-Packard 5890A, was equipped with a capillary column. The column was followed by a ^{63}Ni electron capture detector (ECD). The splitting valve was used on occasion to test the purity of new purchases of radiochemicals. The valve provided the capability of diverting most of the flow (99%) away from the detector in these instances, when a relatively concentrated and radioactive injection was applied. For quantitative purposes, 2-7 μL injections of the pentane were applied, and much less of the flow (<5%) was diverted from the detector. The carrier and makeup gases were helium and Argon/Methane, respectively. The system operated at 150 degrees Celsius, with the detector slightly higher-- 160 degrees Celsius.

5.3.2.3 Radiochemical Purity

Prior to spiking procedures, spiking solutions were routinely analyzed for volatile impurities via the gas chromatography procedures described in the preceding section. No extraneous peaks were detected in analyses with the PCE spiking solutions.

Spiking solutions were routinely tested for ^{14}C-nonvolatile and ^{14}C-CO_2 fractions using an acid/base purging procedure (Lanzarone and McCarty, 1988). The nonvolatile impurities, which were not identified, were found to represent approximately 1-2% of the activity, for the PCE. This fraction appeared to remain in the aqueous phase (i.e., did not sorb) in samples for which the A-B-N test was performed prior to purging. No significant fraction of ^{14}C-CO_2 was detected in the PCE spiking solutions. The equilibrium measurement of the sample supernatant was adjusted downward to account for the nonvolatile fraction.

5.3.3 Column Experiment Protocol

5.3.3.1 Preliminary Preparation

Calibrate the scintillation counting machine (Beckman LS600, Fullerton, CA). At the quarternary HPLC pump, fill the water tank with distilled water (reservoir B) and fill the methanol tank with methanol (reservoir C). Degas the water and methanol tanks with helium for a 1/2 hour. Turn on helium gas at main tank valve and the brass toggle valve that branches to the Teflon tubing to the quarternary HPLC pump. Turn on the helium flow at the pump and get a flow of helium bubbles in the reservoirs. During degassing, continue lab preparation. Label vials (1 through 40) and fill with 5 mL of scintillation cocktail. Record the weight of each of the 40 vials before the experiment begins.

5.3.3.2 Solute Preparation

Retrieve the ^{14}C-labeled PCE or the ^{14}C-labeled methanol sample from the refrigerator and allow the sample to equilibrate at ambient temperature. A glass syringe (Hamilton, Reno, NV) was used to load 10 μL of PCE (or 50 μL of methanol) into the 10 mL syringe pump (filled with degassed water or precise methanol/water mixture). Preliminary tests indicated that these amounts were sufficient solute inputs. All syringes should be cleaned using a double-acetone wash procedure after each use. Mix the ^{14}C-labeled solute input (10 mL syringe pump spiked with radio-labeled PCE or radio-labeled methanol) over a magnetic mixer. Replace sample caps with new teflon caps.

Find C_o (initial concentration in syringe pump). Using three vials labeled A, B, and C; manually, via a syringe, load 5 μL of the radio-labeled 10 mL sample into each of the three vials. Cap and shake immediately. This procedure is performed three times (A, B, & C) to account for possible non-uniform mixing in the syringe pump. Clean the syringe with the double-acetone wash procedure after each sample: A, B, & C. Using the counting machine, obtain a "quick dpm (disintegrations per minute) count" on A, B, & C vials to verify a uniform C_o. A "quick dpm count" means the counting machine, using a smaller sample time, will give a dpm count that still maintains a relative error that is less than 2%. The initial concentration is calculated by finding the average of the concentrations of A, B, and C.

When the three counts are within 5% of each other, proceed with the experiment. Set the quarternary HPLC pump to the desired flow rate (0.745 ml/min) and desired methanol/water mixture (0%, 1%, 5%, 10%, 20%, or 50%). Load empty vials 1 through 40 in the auto sampler (Isis Autosampler, Lincoln, NE). Load about three rows of empty test vials in the auto sampler. Set sample and wash times on the auto sampler (i.e., 20 seconds sample interval and one minute 35 seconds wash time).

5.3.3.3 Lab

Record start time of the experiment. Actuate the syringe pump to load the step input into the column. When the syringe is completely empty, turn-off syringe pump, switch the actuator, and engage the quarternary HPLC pump. Note the time the pulse was stopped. This is the length of the step input. Note the time when the supply of test vials is exhausted and the time when the first recorded sample is taken.

While the experiment is in progress, monitor the quarternary HPLC pump for stoppages. Note the time of any mishaps during the experiment run. Continue to sample the remaining 39 vials. Cap and shake each vial after every sample is taken. Rinse sample tube after each sample vial is taken using distilled water. At the end of the experiment, note the time of completion. After the last sample, turn off the auto sampler while the sampling rod is in the washing tube.

5.3.3.4 Post-Lab

Weigh each of the 40 sample vials. Load the A, B, C vials and the 40 sample vials into the scintillation counter. Program the counting machine to count the dpm's (ten minute counting time, twice each vial). The packed column must be flushed completely with degassed water before another experiment is run (preferably the next day). When flushing the column, ensure the packed column is in the vertical position. Turn off helium sources at the HPLC pump and the helium tank. Turn off all machines. Clean-up counters and police the area.

5.4 Data Reduction

The data from the scintillation counter will give the "dpm count" for each of the sample vials. The "dpm count" is a mass measurement. To be used in the CFITM model,

the mass measurement must be converted to a concentration measurement. Each "dpm count" will be divided by the difference between the final and initial weights of each corresponding sample vial. The difference between the final and initial weight of each sample vial is in the units of grams. To convert this difference measurement to mLs, divide by the density of water (≅ 1 g/mL). The "dpm/mL" measurement is now in concentration (aqueous) units. All data reduction spreadsheets are included in Appendix A, Column Run Spreadsheets.

5.5 CFITM Model Input

The data input for the model for each sample vial is equivalent "pore volume" [-], and corresponding sample concentration (in [dpm/mL]; as calculated in section 5.4). CFITM provides a least-squares fit for each experimental data point. This output, when connected, is the fitted curve for the column effluent data.

The CFITM data input files for each of the column runs is shown in Appendix B, CFITM Data Input.

5.6 Expected Shape of Breakthrough Curves

The processes affecting solute transport in the saturated zone are advection and hydrodynamic dispersion. Advection would carry the dissolved chemical with the groundwater flow. In an ideal porous media, it would produce close to "plug flow" behavior. Hydrodynamic dispersion would cause the dissolved chemical to spread throughout the porous media. The curves in Figure 5-2 show the shape of the expected breakthrough curve given a square pulse input of solute.

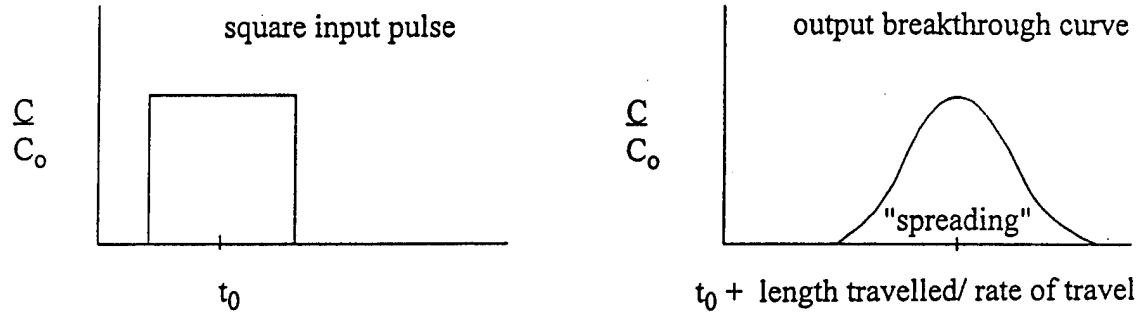

Figure 5-2. Expected output breakthrough curve given a square input pulse.

In Figure 5-2, t_0 is the corresponding time for the center mass of the square input pulse. The degree of "spreading" in the output breakthrough curve varies according to the amount of hydrodynamic dispersion. As shown on the time-scale of the output breakthrough curve, the arrival time of the peak is a function of the length of and the rate at which the input pulse travels.

Chapter 6. Results and Discussion

6.1 Overview

Specific results are described in the following sections. Section 6.2 presents column breakthrough data for the miscible displacement tests; that is, employing methanol or PCE as single solutes. Section 6.3 presents the results for the methanol slug tests in which cosolvent levels of methanol were used to displace water from the column. Section 6.4 presents the PCE breakthrough curves subject to MeOH cosolvent levels. Throughout Chapter 6, the breakthrough data are plotted along with CFITM model output derived from the curve fitting protocols discussed in Section 5.5. Output from the CFITM program for each column run is included in Appendix C, CFITM Data Output.

The breakthrough curves for each of the column runs are shown in the following sections. As discussed previously in Section 5.6, all of the breakthrough curves are similar in shape to the output curves shown in Figure 5-2.

6.2 Miscible Displacement Results: Methanol and PCE

The first two sets of column experiments were tracer studies employing dilute amounts of either ^{14}C-labeled MeOH or ^{14}C-labeled PCE. In each case, the input pulse contained no methanol (0% methanol fraction). The purpose of the tracers was to provide a basis for comparison of the methanol displacement experiments and the PCE mobilization experiments. Figure 6-1 shows the tracer run for the ^{14}C-labeled MeOH. Figure 6-2 shows the tracer run for the ^{14}C-labeled PCE.

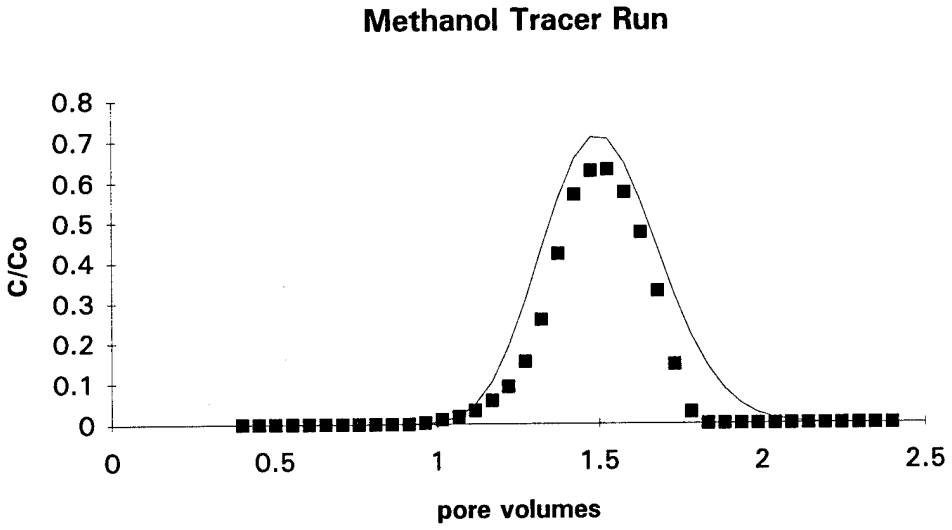

Figure 6-1. Methanol tracer breakthrough curve for a 0.745 mL/min flowrate.

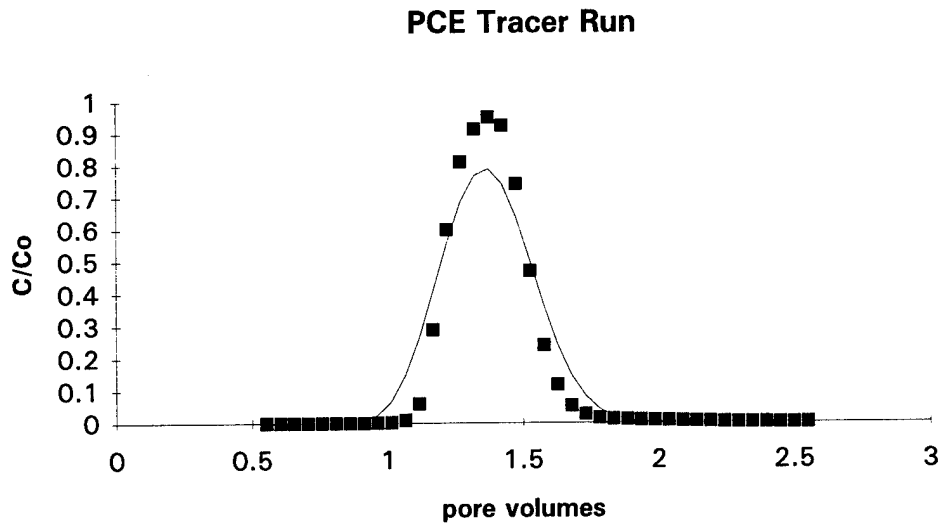

Figure 6-2. PCE tracer breakthrough curve for a 0.745 mL/min flowrate.

The solid squares on Figure 6-1 and Figure 6-2 represent the experimental data. The solid line represents CFITM's best-fitting curve, using a Peclet number equal to 159. A summary of the methanol and PCE tracer tests are shown below in Table 6-1.

Column Run	Methanol (%)	Flow (mL/min)	Peclet Number	Retardation Factor	95% Confidence Limit	
					Lower	Upper
Tracer MeOH	0	0.745	***159***	1.00	112	206
Tracer PCE	0	0.745	159	***1.20***	1.18	1.22

Table 6-1. Summary of Methanol and PCE Tracer Runs.

Note- Numbers in bold italics indicate fitted data.

For each of the methanol tracer runs, the breakthrough curve begins to appear at approximately one pore volume. The expectation is that the center of the breakthrough curve should elute at one pore volume plus half of the total length of the input pulse (also in pore volumes). The center of the methanol tracer breakthrough curve occurs, for each tracer run, at approximately 1.5 pore volumes. The peaks arrive slightly later than expected; however, considering experimental error, the tracer curves show that the methanol was transported with the pore water, and not retarded.

The experimental tracer runs exhibited predictable behavior. The 0.745 mL/min flow rate used in each of the column runs was a relatively fast flow rate as shown by the shape of the breakthrough curves. The sharpness of the front and elution portions of the curves were indicative of advection dominated transport characteristic of a high Peclet number.

6.3 MeOH Displacement Experiments

The objective of the second set of column experiments was to characterize the advection and dispersion behavior of methanol as a cosolvent. More specifically, the purpose was to characterize the extent that methanol displacing water behaved immiscibly, due to density and viscosity differences. The methanol fractions tested (1%, 5%, 10%, 20%, and 50% v/v) exhibited similar behavior. Figures 6-3 through 6-7 show the methanol breakthrough curves for the 1%, 5%, 10%, 20%, and 50% methanol fractions respectively.

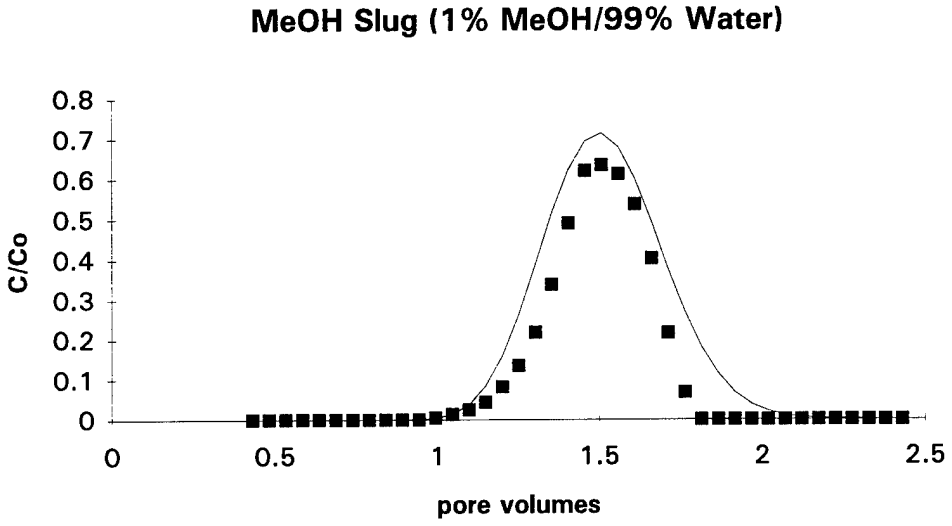

Figure 6-3. 1% MeOH slug breakthrough at a 0.745 mL/min flowrate.

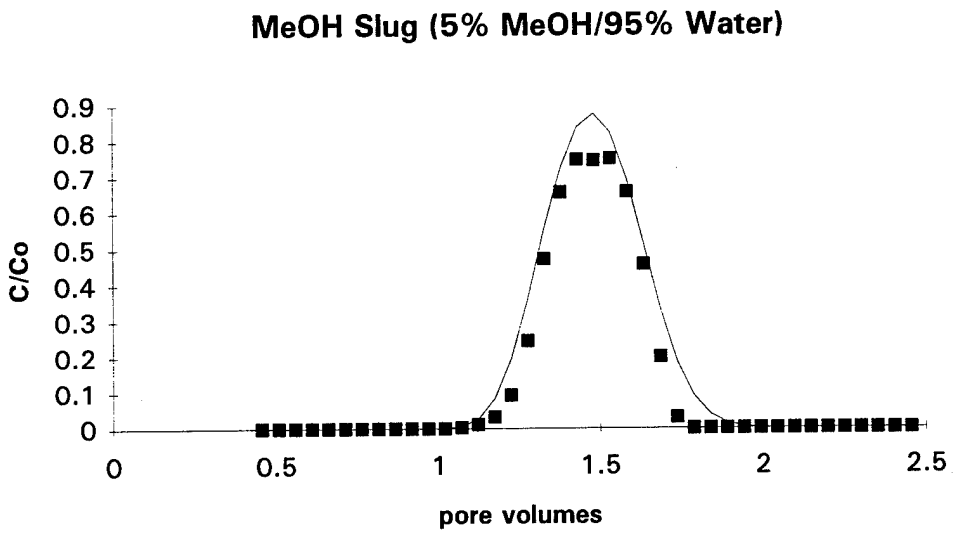

Figure 6-4. 5% MeOH slug breakthrough at a 0.745 mL/min flowrate.

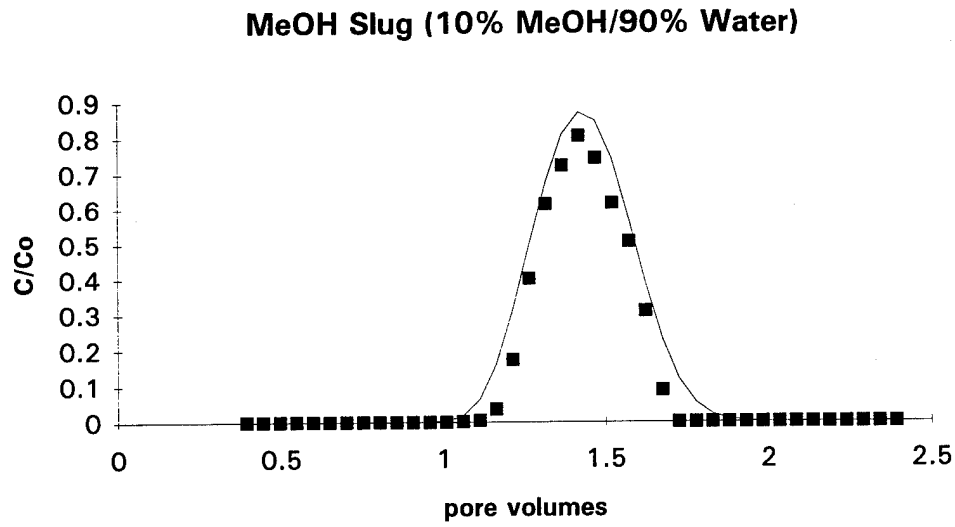

Figure 6-5. 10% MeOH slug breakthrough at a 0.745 mL/min flowrate.

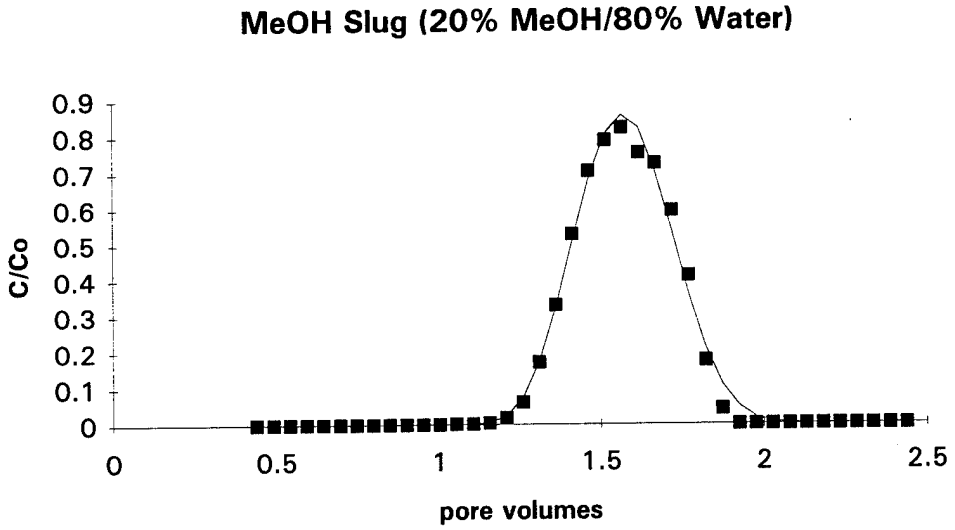

Figure 6-6. 20% MeOH slug breakthrough at a 0.745 mL/min flowrate.

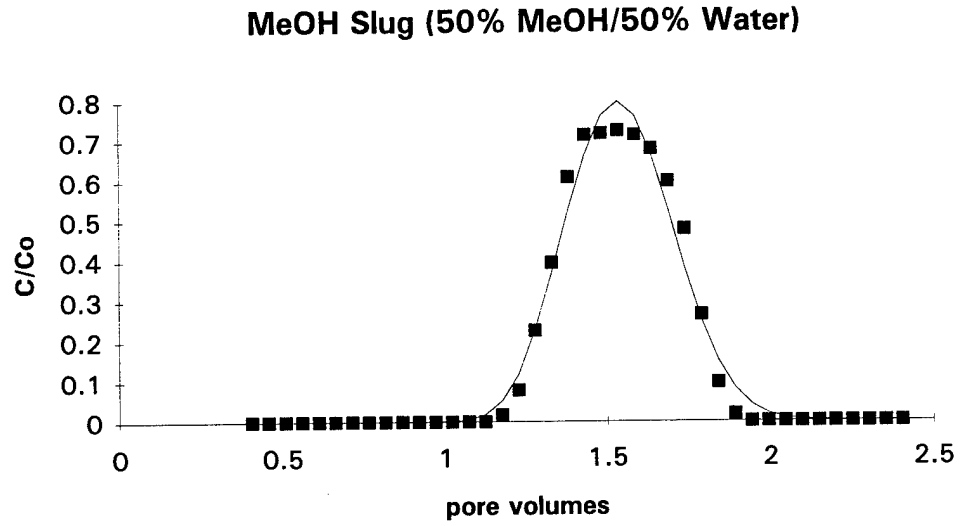

Figure 6-7. 50% MeOH slug breakthrough at a 0.745 mL/min flowrate.

The simulation providing the best-fit for the data was characterized by a Peclet number of 328, the resulting Peclet number for the 20% MeOH fraction. Each of the column runs

had similar square mass inputs (pulses). When calculating the area below each of the output curves, it was estimated that at least 93% of the mass input was conserved for each column run (Appendix A, Column Run Spreadsheets).

Each of the column runs produced breakthrough curves that were characteristic of advection dominated transport. Analysis of the breakthrough curves shows that there was no evidence of unstable fronts nor was there evidence of "over-riding" or "wedging" of methanol over water. Table 6-2 summarizes the results of the MeOH slug experiments.

Column Run	Methanol (%)	Flow (mL/min)	Peclet Number	Retardation Factor	95% Confidence Limit	
					Lower	Upper
MeOH Slug	1	0.745	***153***	1.00	106	200
MeOH Slug	5	0.745	***305***	1.00	224	385
MeOH Slug	10	0.745	***276***	1.00	199	352
MeOH Slug	20	0.745	***328***	1.00	293	364
MeOH Slug	50	0.745	***221***	1.00	190	253

Table 6-2. Summary of MeOH Slug Experiments.

Note- Numbers in bold italics indicate fitted data.

The MeOH slug run at 1% methanol by volume was characterized by a Peclet number similar to that of the MeOH tracer run. However, the methanol runs with greater methanol percentages by volume were characterized by significantly larger Peclet numbers. The sharpness of the corresponding curve fronts were also indicative of the larger Peclet numbers. Each of the methanol runs exhibited early breakthrough, however,

this was due to improperly flushing the radio-labeled MeOH from the previous column experiments. An adjusted C/C_0 value was calculated to correct for this inaccuracy.

6.4 PCE Mobilization Breakthrough Curves

The final set of experiments determined the effect of different methanol fractions on the mobilization of PCE in the soil column. Again, the methanol fractions tested (1%, 5%, 10%, 20%, and 50% v/v) exhibited similar behavior. From the output curves, one would expect that with increasing methanol fraction, the curves would exhibit earlier breakthrough, indicative of a decrease of the retardation factor of PCE. Figures 6-8 through 6-12 show the PCE mobilization breakthrough curves for each of the methanol fractions.

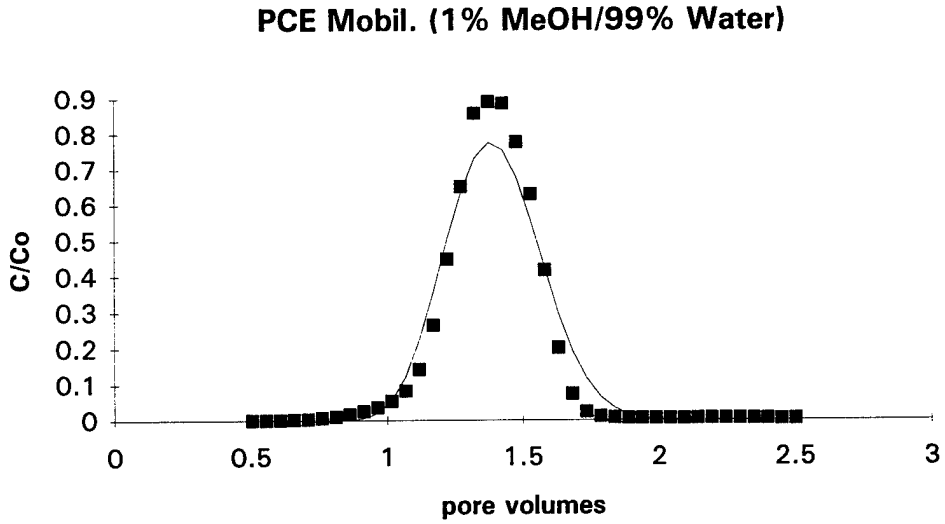

Figure 6-8. PCE mobilization breakthrough (1% MeOH) at a 0.745 mL/min flowrate.

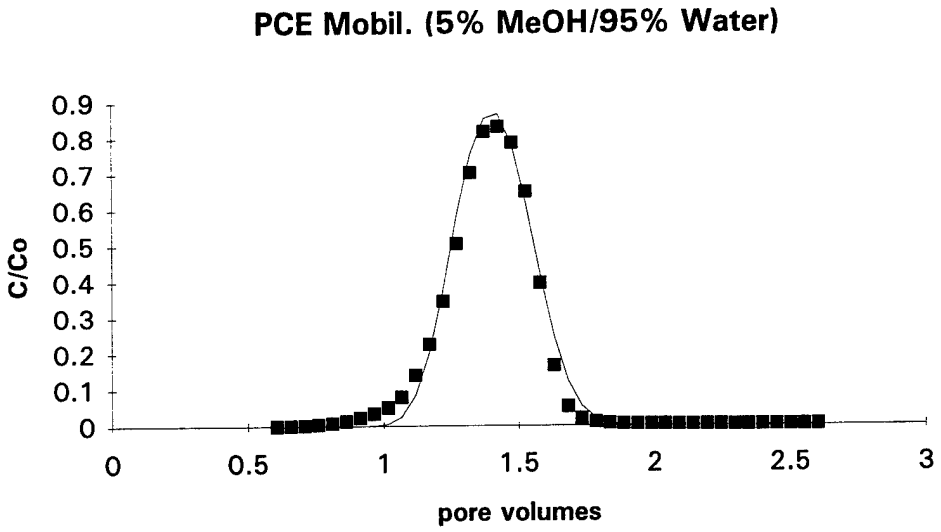

Figure 6-9. PCE mobilization breakthrough (5% MeOH) at a 0.745 mL/min flowrate.

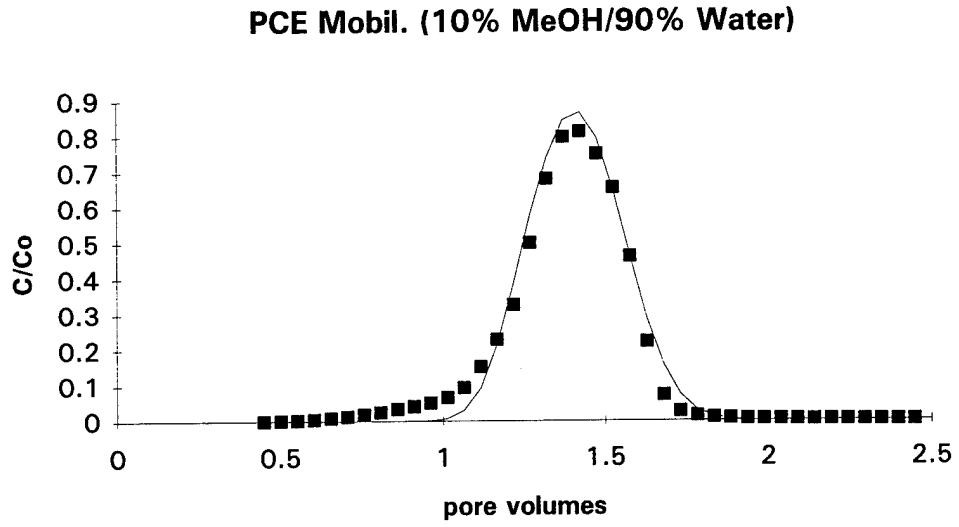

Figure 6-10. PCE mobilization breakthrough (10% MeOH) at a 0.745 mL/min flowrate.

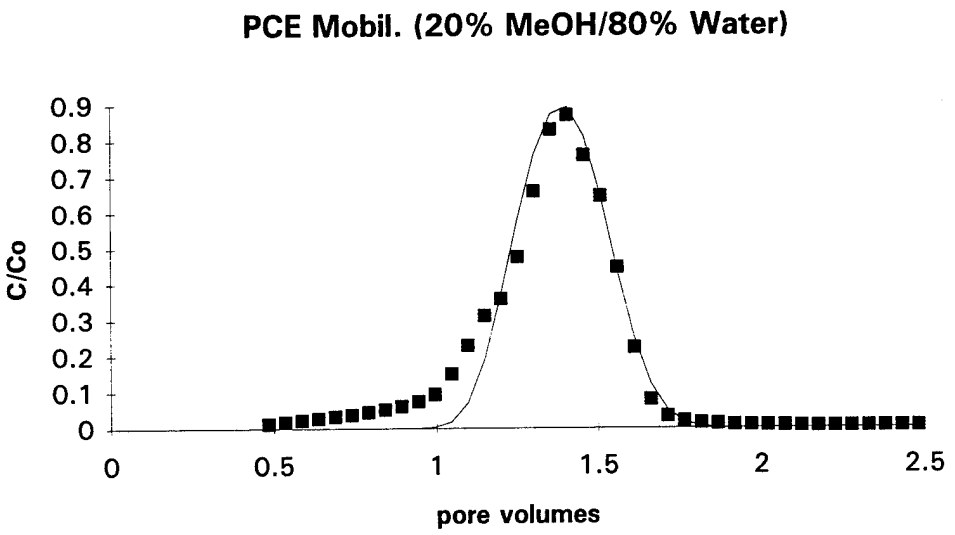

Figure 6-11. PCE mobilization breakthrough (20% MeOH) at a 0.745 mL/min flowrate.

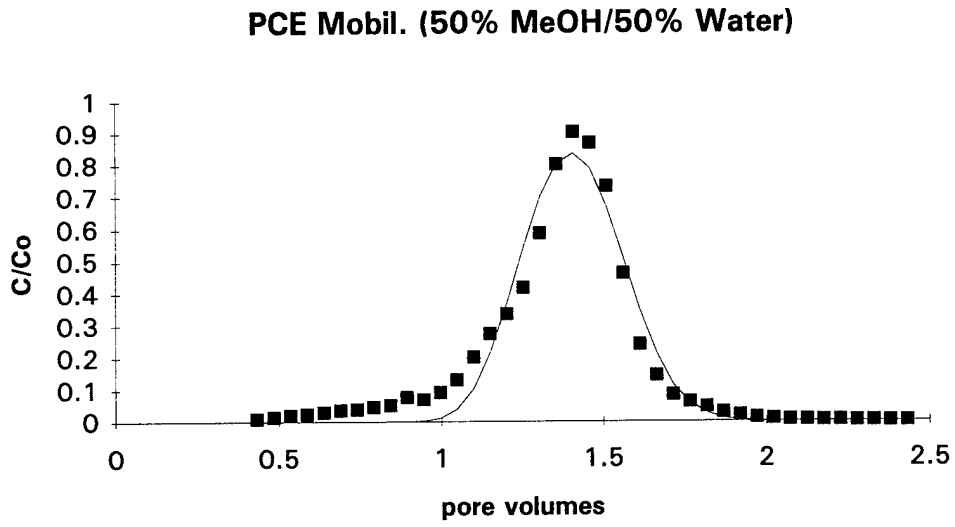

Figure 6-12. PCE mobilization breakthrough (50% MeOH) at a 0.745 mL/min flowrate.

All of the PCE retardation results (1%, 5%, 10%, 20%, and 50%) were similar. As with the MeOH slug runs, each of the PCE mobilization column runs produced breakthrough

curves that were characteristic of advection dominated transport. The simulation providing the best-fit for the data was characterized by a retardation factor of 1.22, corresponding to the 20% MeOH fraction. Each of the column runs had similar square mass inputs (pulses). When calculating the area below each of the output curves, it was estimated that at least 97% of the mass input was conserved for each column run. Table 6-3 summarizes the PCE retardation results.

Column Run	Methanol (%)	Flow (mL/min)	Peclet Number	Retardation Factor	95% Confidence Limit	
					Lower	Upper
PCE Input	1	0.745	153	***1.22***	1.21	1.24
PCE Input	5	0.745	305	***1.25***	1.25	1.26
PCE Input	10	0.745	276	***1.25***	1.24	1.26
PCE Input	20	0.745	328	***1.23***	1.22	1.24
PCE Input	50	0.745	221	***1.24***	1.23	1.25

Table 6-3. Summary of PCE Retardation Experiments.

Note- Numbers in bold italics indicate fitted data.

In general, the PCE breakthrough curves were symmetrical and weakly retarded. The PCE runs with 20% methanol and 50% methanol each exhibited slightly early breakthrough and slight tailing.

Van Genuchten's Least Squares Program determined the best-fitting retardation factor for each of the observed breakthrough curves. All of the resulting retardation factors are plotted in Figure 6-13 as a function of the methanol fraction.

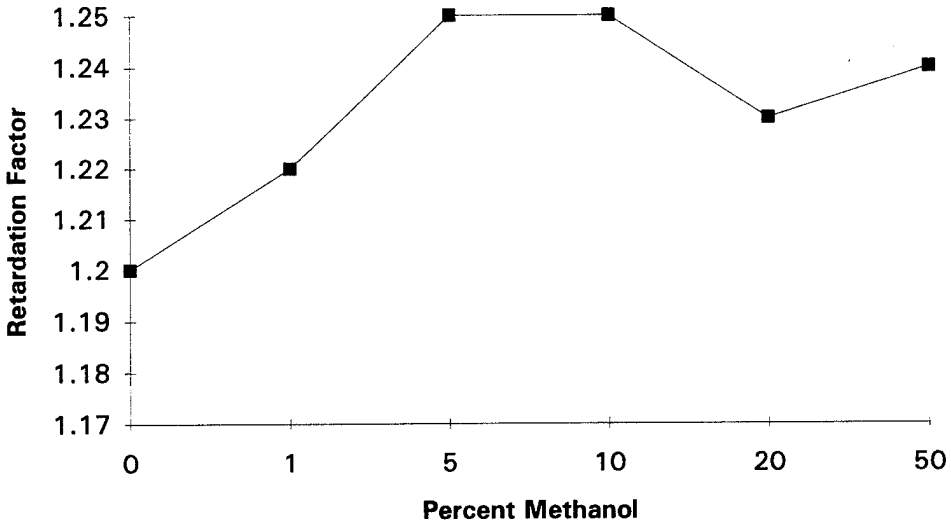

Figure 6-13. Retardation Factors with respect to methanol fractions.

The results do not indicate any trends. The retardation factor only varied between 1.20 and 1.25. Essentially, there was no significant difference in retardation factor with increasing methanol fraction.

The PCE mobilization experiments failed to demonstrate the hypothesized results. The degree of retardation of PCE did not decrease log-linearly with increasing methanol fraction. However, the results of this study confirmed the results of previous studies (Imhoff, 1995). The MeOH slug experiments showed that with an increasing methanol fraction, there was an increase in the Peclet number.

Chapter 7. Summary and Conclusions

The goal of this research was to test the ability of methanol as an effective cosolvent. This study investigated the transport and dissolution of methanol in a water-saturated porous medium and the effects of methanol on the mobilization of PCE. 1-D column experiments were used to examine: the transport behavior of trace amounts of ^{14}C-labeled methanol/PCE in water; the transport of various methanol fractions through a sand column; and, methanol mobilizing PCE in a saturated soil column.

The one-dimensional column apparatus devised for this work performed adequately. An average of 95% of the mass input through the column was calculated in the mass output indicating that a majority of the mass was conserved. The tracer and slug breakthrough curves of the methanol were described well by the advection/dispersion equation, and showed no indications of density and viscosity difference effects.

For the 1-D laboratory column at the flowrate tested (0.745 mL/min), methanol failed to produce the hypothesized cosolvent effect in mobilizing PCE. Two possible reasons for this failure exist: (1) The PCE sorbed too weakly to the porous medium and any reductions in the sorption were difficult to observe given the experimental uncertainty produced by the methods; (2) The MeOH front by-passed much of the porous medium, thereby failing to mix sufficiently in a timely manner. Given the apparent stability of the methanol slug breakthrough curves, the first reason appears to be the more likely of the two.

Further studies on flow conditions in a contaminated region need to be investigated. Perhaps the 0.745 mL/min flow rate used in this study was too fast to adequately demonstrate the impact of methanol on sorption rates. Although the outcome of this research was not completely as expected, the results do provide motivation for future work to address these flow and transport issues.

Appendix A. Column Run Spreadsheets

Explanation of Terms for Spreadsheets-

__/__%: Type of column run. First number refers to MeOH fraction; second number refers to percent water.

flow: flow rate at which the experiment was conducted.

time: the time at which the sample was completed. For each of the column runs, the sample time in the vial was 20 seconds, the wash time in the waste stream was 100 seconds, and the time in between sampling and washing was 3 seconds. Total time between sampling vials was 123 seconds (2 minutes, 3 seconds).

conv.: time conversion to decimals.

pore vol.: time conversion to equivalent, unitless "pore volumes."

dpm: "disintegrations per minute" as recorded by the scintillation counter. (dpm = concentration [C]).

diff: Difference in weight [g] between the sample vial initially and the sample vial after sampling.

dpm/diff: Self-explanatory. Assuming the density of water is 1 g per cm^3, [dpm/mL].

Co: Initial concentration of input pulse [dpm/mL].

C/Co: Dimensionless parameter [sample concentration/initial concentration].

Adj C/Co: Adjusted C/Co value to account for inaccuracies caused by insufficient column flushing [-].

M: Mass of radio-labeled MeOH or PCE in the sample vial [dpm].

Mo: Initial mass of input pulse [dpm].

M/Mo: Dimensionless parameter [sample mass/total initial mass].

CFIT: Fitted value by van Genuchten's model based on experimental output [dpm/mL].

0/100%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	Adj C/Co	M	Mo	M/Mo		pore vol.	CFIT
meth	0:16:00	16	0.4	2352.17	0.28218	8335.708	184149.3	0.045266	-0.00473	12730.71	1749188	0.007278		0.4	0
tracer	0:18:03	18.05	0.45125	2741.78	0.27514	9965.036	184149.3	0.054114	0.004114	15219.1	1749188	0.008701		0.45125	0
	0:20:06	20.1	0.5025	3187.25	0.29624	10759.01	184149.3	0.058425	0.008425	16431.7	1749188	0.009394		0.5025	0
flow	0:22:09	22.15	0.55375	2707.42	0.2523	10730.96	184149.3	0.058273	0.008273	16388.85	1749188	0.009369		0.55375	0
0.745	0:24:12	24.2	0.605	3007.02	0.2978	10097.45	184149.3	0.054833	0.004833	15421.33	1749188	0.008816		0.605	0
(mL/min)	0:26:15	26.25	0.65625	2692.45	0.28399	9480.792	184149.3	0.051484	0.001484	14479.54	1749188	0.008278		0.65625	0
	0:28:18	28.3	0.7075	2700.31	0.29565	9133.469	184149.3	0.049598	-0.0004	13949.09	1749188	0.007975		0.7075	0
	0:30:21	30.35	0.75875	2422.26	0.26239	9231.526	184149.3	0.050131	0.000131	14098.85	1749188	0.00806		0.75875	0
	0:32:24	32.4	0.81	2654.62	0.29869	8887.542	184149.3	0.048263	-0.00174	13573.5	1749188	0.00776		0.81	0
	0:34:27	34.45	0.86125	2475.85	0.28079	8817.444	184149.3	0.047882	-0.00212	13466.44	1749188	0.007699		0.86125	0
	0:36:30	36.5	0.9125	2729.84	0.30155	9052.694	184149.3	0.04916	-0.00084	13825.73	1749188	0.007904		0.9125	0
	0:38:33	38.55	0.96375	2834.39	0.29127	9731.143	184149.3	0.052844	0.002844	14861.89	1749188	0.008496		0.96375	0.001
	0:40:36	40.6	1.015	3256.88	0.28962	11245.36	184149.3	0.061067	0.011067	17174.47	1749188	0.009819		1.015	0.006
	0:42:39	42.65	1.06625	3524.05	0.27962	12603	184149.3	0.068439	0.018439	19247.93	1749188	0.011004		1.06625	0.018
	0:44:42	44.7	1.1175	4402.99	0.29154	15102.52	184149.3	0.082012	0.032012	23065.33	1749188	0.013186		1.1175	0.048
	0:46:45	46.75	1.16875	5379.17	0.27474	19579.13	184149.3	0.106322	0.056322	29902.23	1749188	0.017095		1.16875	0.103
	0:48:48	48.8	1.22	6793.25	0.26143	25984.97	184149.3	0.141108	0.091108	39685.54	1749188	0.022688		1.22	0.189
	0:50:51	50.85	1.27125	10285.85	0.2756	37321.66	184149.3	0.202671	0.152671	56999.51	1749188	0.032586		1.27125	0.303
	0:52:54	52.9	1.3225	16182.19	0.28659	56464.6	184149.3	0.306624	0.256624	86235.56	1749188	0.0493		1.3225	0.434
	0:54:57	54.95	1.37375	22785.14	0.263	86635.51	184149.3	0.470463	0.420463	132314.1	1749188	0.075643		1.37375	0.558
	0:57:00	57	1.425	32800.14	0.28845	113711.7	184149.3	0.617497	0.567497	173666.2	1749188	0.099284		1.425	0.656
	0:59:03	59.05	1.47625	35488.19	0.2851	124476.3	184149.3	0.675953	0.625953	190106.4	1749188	0.108683		1.47625	0.708
	1:01:06	61.1	1.5275	33544.8	0.26831	125022.5	184149.3	0.678919	0.628919	190940.7	1749188	0.10916		1.5275	0.704
	1:03:09	63.15	1.57875	32803.06	0.28581	114772.3	184149.3	0.623256	0.573256	175285.9	1749188	0.10021		1.57875	0.646
	1:05:12	65.2	1.63	28218.48	0.29288	96348.27	184149.3	0.523207	0.473207	147147.9	1749188	0.084124		1.63	0.55
	1:07:15	67.25	1.68125	19814.25	0.28503	69516.37	184149.3	0.3775	0.3275	106168.9	1749188	0.060696		1.68125	0.435
	1:09:18	69.3	1.7325	10091.8	0.28028	36006.14	184149.3	0.195527	0.145527	54990.37	1749188	0.031438		1.7325	0.318
	1:11:21	71.35	1.78375	4031.68	0.27924	14438.05	184149.3	0.078404	0.028404	22050.51	1749188	0.012606		1.78375	0.219
	1:13:24	73.4	1.835	1401.85	0.26025	5386.551	184149.3	0.029251	-0.02075	8226.611	1749188	0.004703		1.835	0.141
	1:15:27	75.45	1.88625	730.66	0.28264	2585.126	184149.3	0.014038	-0.03596	3948.134	1749188	0.002257		1.88625	0.086
	1:17:30	77.5	1.9375	562.14	0.28621	1964.082	184149.3	0.010666	-0.03933	2999.645	1749188	0.001715		1.9375	0.049
	1:19:33	79.55	1.98875	433.23	0.25932	1670.639	184149.3	0.009072	-0.04093	2551.483	1749188	0.001459		1.98875	0.026
	1:21:36	81.6	2.04	435.98	0.28769	1515.451	184149.3	0.008229	-0.04177	2314.472	1749188	0.001323		2.04	0.014
	1:23:39	83.65	2.09125	377.34	0.2784	1355.388	184149.3	0.00736	-0.04264	2070.016	1749188	0.001183		2.09125	0.007
	1:25:42	85.7	2.1425	352.89	0.28682	1230.354	184149.3	0.006681	-0.04332	1879.057	1749188	0.001074		2.1425	0.003
	1:27:45	87.75	2.19375	309.22	0.29346	1053.704	184149.3	0.005722	-0.04428	1609.27	1749188	0.00092		2.19375	0.001
	1:29:48	89.8	2.245	269.96	0.2791	967.2519	184149.3	0.005253	-0.04475	1477.235	1749188	0.000845		2.245	0.001
	1:31:51	91.85	2.29625	241.06	0.27528	875.6902	184149.3	0.004755	-0.04524	1337.398	1749188	0.000765		2.29625	0
	1:33:54	93.9	2.3475	224.67	0.29142	770.9491	184149.3	0.004187	-0.04581	1177.432	1749188	0.000673		2.3475	0
	1:35:57	95.95	2.39875	209.46	0.29172	718.0173	184149.3	0.003899	-0.0461	1096.592	1749188	0.000627		2.39875	0
										1670116		0.954795			

1/99%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	Adj C/Co	M	Mo	M/Mo		pore vol.	CFIT
meth	0:17:15	17.25	0.43125	3121.88	0.27801	11229.38	230856	0.048642	-0.00136	17150.07	2235840	0.007671		0.43125	0
slug	0:19:18	19.3	0.4825	3674.83	0.28193	13034.55	230856	0.056462	0.006462	19907.01	2235840	0.008904		0.4825	0
	0:21:21	21.35	0.53375	3697.04	0.2748	13453.57	230856	0.058277	0.008277	20546.96	2235840	0.00919		0.53375	0
flow	0:23:24	23.4	0.585	3796.5	0.30203	12569.94	230856	0.054449	0.004449	19197.45	2235840	0.008586		0.585	0
0.745	0:25:27	25.45	0.63625	3512.64	0.28971	12124.68	230856	0.052521	0.002521	18517.41	2235840	0.008282		0.63625	0
(mL/min)	0:27:30	27.5	0.6875	3261.61	0.2771	11770.52	230856	0.050986	0.000986	17976.52	2235840	0.00804		0.6875	0
	0:29:33	29.55	0.73875	3053.51	0.27453	11122.68	230856	0.04818	-0.00182	16987.12	2235840	0.007598		0.73875	0
	0:31:36	31.6	0.79	3170.53	0.29584	10717.04	230856	0.046423	-0.00358	16367.6	2235840	0.007321		0.79	0
	0:33:39	33.65	0.84125	3199.38	0.30043	10649.34	230856	0.04613	-0.00387	16264.2	2235840	0.007274		0.84125	0
	0:35:42	35.7	0.8925	3206.62	0.29939	10710.51	230856	0.046395	-0.00361	16357.63	2235840	0.007316		0.8925	0
	0:37:45	37.75	0.94375	3601.85	0.31185	11549.94	230856	0.050031	3.09E-05	17639.65	2235840	0.007889		0.94375	0.001
	0:39:48	39.8	0.995	3707.97	0.29429	12599.71	230856	0.054578	0.004578	19242.91	2235840	0.008607		0.995	0.004
	0:41:51	41.85	1.04625	3972.68	0.27078	14671.25	230856	0.063552	0.013552	22406.66	2235840	0.010022		1.04625	0.014
	0:43:54	43.9	1.0975	5170.31	0.30059	17200.54	230856	0.074508	0.024508	26269.52	2235840	0.011749		1.0975	0.037
	0:45:57	45.95	1.14875	6813.97	0.31523	21615.87	230856	0.093634	0.043634	33012.83	2235840	0.014765		1.14875	0.084
	0:48:00	48	1.2	9274.81	0.30432	30477.16	230856	0.132018	0.082018	46546.25	2235840	0.020818		1.2	0.159
	0:50:03	50.05	1.25125	10656.11	0.24923	42756.13	230856	0.185207	0.135207	65299.3	2235840	0.029206		1.25125	0.262
	0:52:06	52.1	1.3025	18798.31	0.30392	61852.82	230856	0.267928	0.217928	94464.72	2235840	0.04225		1.3025	0.388
	0:54:09	54.15	1.35375	25062.83	0.27956	89650.99	230856	0.388342	0.338342	136919.5	2235840	0.061238		1.35375	0.515
	0:56:12	56.2	1.405	36976.07	0.2969	124540.5	230856	0.539473	0.489473	190204.5	2235840	0.085071		1.405	0.623
	0:58:15	58.25	1.45625	45216.18	0.2926	154532.4	230856	0.669389	0.619389	236009.6	2235840	0.105557		1.45625	0.694
	1:00:18	60.3	1.5075	43849.62	0.27775	157874.4	230856	0.683865	0.633865	241113.7	2235840	0.10784		1.5075	0.714
	1:02:21	62.35	1.55875	43856.55	0.28728	152661.3	230856	0.661284	0.611284	233152	2235840	0.104279		1.55875	0.68
	1:04:24	64.4	1.61	39251.06	0.28994	135376.5	230856	0.586411	0.536411	206753.7	2235840	0.092472		1.61	0.601
	1:06:27	66.45	1.66125	29087.4	0.27819	104559.5	230856	0.452921	0.402921	159688.5	2235840	0.071422		1.66125	0.494
	1:08:30	68.5	1.7125	20156.22	0.328	61451.89	230856	0.266191	0.216191	93852.4	2235840	0.041976		1.7125	0.377
	1:10:33	70.55	1.76375	8548.3	0.31434	27194.44	230856	0.117798	0.067798	41532.71	2235840	0.018576		1.76375	0.27
	1:12:36	72.6	1.815	2656.38	0.28023	9479.285	230856	0.041061	-0.00894	14477.24	2235840	0.006475		1.815	0.182
	1:14:39	74.65	1.86625	1208.53	0.31282	3863.34	230856	0.016735	-0.03327	5900.286	2235840	0.002639		1.86625	0.115
	1:16:42	76.7	1.9175	698.21	0.28843	2420.726	230856	0.010486	-0.03951	3697.054	2235840	0.001654		1.9175	0.068
	1:18:45	78.75	1.96875	562.67	0.29034	1937.969	230856	0.008395	-0.04161	2959.764	2235840	0.001324		1.96875	0.039
	1:20:48	80.8	2.02	461.87	0.28363	1628.424	230856	0.007054	-0.04295	2487.011	2235840	0.001112		2.02	0.021
	1:22:51	82.85	2.07125	393.61	0.29187	1348.58	230856	0.005842	-0.04416	2059.619	2235840	0.000921		2.07125	0.011
	1:24:54	84.9	2.1225	350.33	0.28569	1226.259	230856	0.005312	-0.04469	1872.804	2235840	0.000838		2.1225	0.005
	1:26:57	86.95	2.17375	304.98	0.27928	1092.022	230856	0.00473	-0.04527	1667.791	2235840	0.000746		2.17375	0.003
	1:29:00	89	2.225	292.26	0.29769	981.7595	230856	0.004253	-0.04575	1499.392	2235840	0.000671		2.225	0.001
	1:31:03	91.05	2.27625	256.34	0.29741	861.9078	230856	0.003734	-0.04627	1316.349	2235840	0.000589		2.27625	0.001
	1:33:06	93.1	2.3275	235.52	0.30255	778.4498	230856	0.003372	-0.04663	1188.888	2235840	0.000532		2.3275	0
	1:35:09	95.15	2.37875	205.92	0.3034	678.708	230856	0.00294	-0.04706	1036.557	2235840	0.000464		2.37875	0
	1:37:12	97.2	2.43	180.13	0.29762	605.2349	230856	0.002622	-0.04738	924.3449	2235840	0.000413		2.43	0
										2084467		0.932297			

5/95%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	Adj C/Co	M	Mo	M/Mo		pore vol.	CFIT
meth	0:18:15	18.25	0.45625	1961.66	0.30121	6512.599	207208	0.03143	-0.01857	9946.367	2006809	0.004956		0.45625	0
slug	0:20:18	20.3	0.5075	2380.78	0.28853	8251.412	207208	0.039822	-0.01018	12601.97	2006809	0.00628		0.5075	0
	0:22:21	22.35	0.55875	2780.3	0.27834	9988.863	207208	0.048207	-0.00179	15255.49	2006809	0.007602		0.55875	0
flow	0:24:24	24.4	0.61	3477.41	0.31543	11024.35	207208	0.053204	0.003204	16836.94	2006809	0.00839		0.61	0
0.745	0:26:27	26.45	0.66125	3114.01	0.27814	11195.84	207208	0.054032	0.004032	17098.84	2006809	0.00852		0.66125	0
(mL/min)	0:28:30	28.5	0.7125	2973.95	0.29027	10245.46	207208	0.049445	-0.00055	15647.38	2006809	0.007797		0.7125	0
	0:30:33	30.55	0.76375	2790.12	0.28472	9799.522	207208	0.047293	-0.00271	14966.32	2006809	0.007458		0.76375	0
	0:32:36	32.6	0.815	2642.07	0.27815	9498.724	207208	0.045841	-0.00416	14506.93	2006809	0.007229		0.815	0
	0:34:39	34.65	0.86625	2820	0.29924	9423.874	207208	0.04548	-0.00452	14392.61	2006809	0.007172		0.86625	0
	0:36:42	36.7	0.9175	2661.3	0.28134	9459.373	207208	0.045652	-0.00435	14446.83	2006809	0.007199		0.9175	0
	0:38:45	38.75	0.96875	2632.9	0.28206	9334.539	207208	0.045049	-0.00495	14256.17	2006809	0.007104		0.96875	0
	0:40:48	40.8	1.02	2643.93	0.26972	9802.499	207208	0.047308	-0.00269	14970.87	2006809	0.00746		1.02	0.001
	0:42:51	42.85	1.07125	2955.27	0.2723	10852.99	207208	0.052377	0.002377	16575.23	2006809	0.008259		1.07125	0.006
	0:44:54	44.9	1.1225	3352.62	0.26606	12600.99	207208	0.060813	0.010813	19244.87	2006809	0.00959		1.1225	0.026
	0:46:57	46.95	1.17375	5125.82	0.30247	16946.54	207208	0.081785	0.031785	25881.6	2006809	0.012897		1.17375	0.083
	0:49:00	49	1.225	8279.97	0.28032	29537.56	207208	0.14255	0.09255	45111.24	2006809	0.022479		1.225	0.194
	0:51:03	51.05	1.27625	16937.52	0.27741	61055.91	207208	0.29466	0.24466	93247.64	2006809	0.046466		1.27625	0.36
	0:53:06	53.1	1.3275	30171.24	0.27897	108152.3	207208	0.52195	0.47195	165175.6	2006809	0.082308		1.3275	0.554
	0:55:09	55.15	1.37875	41412.09	0.28258	146550	207208	0.70726	0.65726	223818.4	2006809	0.111529		1.37875	0.724
	0:57:12	57.2	1.43	45529.53	0.27524	165417.6	207208	0.798316	0.748316	252634	2006809	0.125888		1.43	0.838
	0:59:15	59.25	1.48125	44188.59	0.26808	164833.6	207208	0.795498	0.745498	251742.1	2006809	0.125444		1.48125	0.875
	1:01:18	61.3	1.5325	45227.63	0.2725	165973	207208	0.800997	0.750997	253482.2	2006809	0.126311		1.5325	0.824
	1:03:21	63.35	1.58375	39982.63	0.27252	146714.5	207208	0.708054	0.658054	224069.7	2006809	0.111655		1.58375	0.693
	1:05:24	65.4	1.635	30932.71	0.29456	105013.3	207208	0.506801	0.456801	160381.5	2006809	0.079919		1.635	0.513
	1:07:27	67.45	1.68625	13818.47	0.26754	51650.11	207208	0.249267	0.199267	78882.63	2006809	0.039307		1.68625	0.332
	1:09:30	69.5	1.7375	4242.49	0.2554	16611.16	207208	0.080167	0.030167	25369.39	2006809	0.012642		1.7375	0.185
	1:11:33	71.55	1.78875	1582.39	0.30033	5268.838	207208	0.025428	-0.02457	8046.832	2006809	0.00401		1.78875	0.091
	1:13:36	73.6	1.84	785.96	0.28855	2723.826	207208	0.013145	-0.03685	4159.963	2006809	0.002073		1.84	0.039
	1:15:39	75.65	1.89125	538.61	0.28998	1857.404	207208	0.008964	-0.04104	2836.72	2006809	0.001414		1.89125	0.015
	1:17:42	77.7	1.9425	340.99	0.25676	1328.05	207208	0.006409	-0.04359	2028.264	2006809	0.001011		1.9425	0.005
	1:19:45	79.75	1.99375	285.84	0.277	1031.913	207208	0.00498	-0.04502	1575.99	2006809	0.000785		1.99375	0.002
	1:21:48	81.8	2.045	215.72	0.26359	818.3922	207208	0.00395	-0.04605	1249.889	2006809	0.000623		2.045	0
	1:23:51	83.85	2.09625	188.79	0.27232	693.2653	207208	0.003346	-0.04665	1058.789	2006809	0.000528		2.09625	0
	1:25:54	85.9	2.1475	175.47	0.29226	600.3901	207208	0.002898	-0.0471	916.9457	2006809	0.000457		2.1475	0
	1:27:57	87.95	2.19875	131.69	0.25303	520.4521	207208	0.002512	-0.04749	794.8605	2006809	0.000396		2.19875	0
	1:30:00	90	2.25	127.32	0.28471	447.1919	207208	0.002158	-0.04784	682.9738	2006809	0.00034		2.25	0
	1:32:03	92.05	2.30125	121.43	0.29551	410.9167	207208	0.001983	-0.04802	627.5726	2006809	0.000313		2.30125	0
	1:34:06	94.1	2.3525	105.63	0.29847	353.9049	207208	0.001708	-0.04829	540.5013	2006809	0.000269		2.3525	0
	1:36:09	96.15	2.40375	90.74	0.28567	317.6392	207208	0.001533	-0.04847	485.1145	2006809	0.000242		2.40375	0
	1:38:12	98.2	2.455	74.31	0.25573	290.5799	207208	0.001402	-0.0486	443.7882	2006809	0.000221		2.455	0
										2035991		1.014541			

10/90%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	Adj C/Co	M	Mo	M/Mo		pore vol.	CFIT
meth	0:15:45	15.75	0.39375	10.43	0.26675	39.1003	208143	0.00019	-0.09981	59.7159	2028782	2.9E-05		0.39375	0
slug	0:17:48	17.8	0.445	17.16	0.28094	61.0807	208143	0.00029	-0.09971	93.28543	2028782	4.6E-05		0.445	0
	0:19:51	19.85	0.49625	73.93	0.29997	246.458	208143	0.00118	-0.09882	376.4029	2028782	0.00019		0.49625	0
flow	0:21:54	21.9	0.5475	236.31	0.26952	876.781	208143	0.00421	-0.09579	1339.064	2028782	0.00066		0.5475	0
0.745	0:23:57	23.95	0.59875	638.07	0.30653	2081.59	208143	0.01	-0.09	3179.109	2028782	0.00157		0.59875	0
(mL/min)	0:26:00	26	0.65	1023.02	0.27701	3693.08	208143	0.01774	-0.08226	5640.256	2028782	0.00278		0.65	0
	0:28:03	28.05	0.70125	1512.37	0.26163	5780.57	208143	0.02777	-0.07223	8828.372	2028782	0.00435		0.70125	0
	0:30:06	30.1	0.7525	2233.84	0.26682	8372.09	208143	0.04022	-0.05978	12786.27	2028782	0.0063		0.7525	0
	0:32:09	32.15	0.80375	2885.55	0.26693	10810.1	208143	0.05194	-0.04806	16509.78	2028782	0.00814		0.80375	0
	0:34:12	34.2	0.855	4036.54	0.29827	13533.2	208143	0.06502	-0.03498	20668.54	2028782	0.01019		0.855	0
	0:36:15	36.25	0.90625	4283.46	0.26988	15871.7	208143	0.07625	-0.02375	24240.09	2028782	0.01195		0.90625	0
	0:38:18	38.3	0.9575	5083.34	0.27238	18662.7	208143	0.08966	-0.01034	28502.57	2028782	0.01405		0.9575	0.001
	0:40:21	40.35	1.00875	5662.96	0.28933	19572.7	208143	0.09403	-0.00597	29892.36	2028782	0.01473		1.00875	0.004
	0:42:24	42.4	1.06	5495.62	0.25925	21198.1	208143	0.10184	0.00184	32374.87	2028782	0.01596		1.06	0.018
	0:44:27	44.45	1.11125	6167.46	0.28476	21658.4	208143	0.10406	0.00406	33077.87	2028782	0.0163		1.11125	0.063
	0:46:30	46.5	1.1625	7334.39	0.26052	28152.9	208143	0.13526	0.03526	42996.5	2028782	0.02119		1.1625	0.16
	0:48:33	48.55	1.21375	15052.7	0.26506	56789.9	208143	0.27284	0.17284	86732.43	2028782	0.04275		1.21375	0.313
	0:50:36	50.6	1.265	28886.4	0.27691	104317	208143	0.50118	0.40118	159317.8	2028782	0.07853		1.265	0.498
	0:52:39	52.65	1.31625	36744.1	0.24763	148383	208143	0.71289	0.61289	226618.2	2028782	0.1117		1.31625	0.676
	0:54:42	54.7	1.3675	45284.1	0.26458	171155	208143	0.82229	0.72229	261396	2028782	0.12884		1.3675	0.81
	0:56:45	56.75	1.41875	51379.9	0.27252	188536	208143	0.9058	0.8058	287942.1	2028782	0.14193		1.41875	0.871
	0:58:48	58.8	1.47	46316	0.26381	175566	208143	0.84349	0.74349	268132.6	2028782	0.13216		1.47	0.848
	1:00:51	60.85	1.52125	39669	0.26615	149048	208143	0.71608	0.61608	227632.8	2028782	0.1122		1.52125	0.741
	1:02:54	62.9	1.5725	36759.8	0.29091	126361	208143	0.60709	0.50709	192985.4	2028782	0.09512		1.5725	0.571
	1:04:57	64.95	1.62375	23588.9	0.27723	85087.9	208143	0.4088	0.3088	129950.6	2028782	0.06405		1.62375	0.388
	1:07:00	67	1.675	10284.6	0.26285	39127.3	208143	0.18798	0.08798	59757.22	2028782	0.02945		1.675	0.231
	1:09:03	69.05	1.72625	3659.91	0.28617	12789.3	208143	0.06144	-0.03856	19532.44	2028782	0.00963		1.72625	0.12
	1:11:06	71.1	1.7775	1205.7	0.26525	4545.52	208143	0.02184	-0.07816	6942.15	2028782	0.00342		1.7775	0.055
	1:13:09	73.15	1.82875	659.86	0.27571	2393.31	208143	0.0115	-0.0885	3655.185	2028782	0.0018		1.82875	0.022
	1:15:12	75.2	1.88	473.33	0.2879	1644.08	208143	0.0079	-0.0921	2510.918	2028782	0.00124		1.88	0.008
	1:17:15	77.25	1.93125	349.07	0.26919	1296.74	208143	0.00623	-0.09377	1980.449	2028782	0.00098		1.93125	0.003
	1:19:18	79.3	1.9825	344.2	0.29353	1172.62	208143	0.00563	-0.09437	1790.888	2028782	0.00088		1.9825	0.001
	1:21:21	81.35	2.03375	290.18	0.27532	1053.97	208143	0.00506	-0.09494	1609.681	2028782	0.00079		2.03375	0
	1:23:24	83.4	2.085	235.91	0.263	896.996	208143	0.00431	-0.09569	1369.937	2028782	0.00068		2.085	0
	1:25:27	85.45	2.13625	208.45	0.27736	751.55	208143	0.00361	-0.09639	1147.805	2028782	0.00057		2.13625	0
	1:27:30	87.5	2.1875	163.46	0.26006	628.547	208143	0.00302	-0.09698	959.9488	2028782	0.00047		2.1875	0
	1:29:33	89.55	2.23875	146.76	0.27245	538.668	208143	0.00259	-0.09741	822.6802	2028782	0.00041		2.23875	0
	1:31:36	91.6	2.29	129	0.27374	471.25	208143	0.00226	-0.09774	719.7167	2028782	0.00035		2.29	0
	1:33:39	93.65	2.34125	105.6	0.27264	387.324	208143	0.00186	-0.09814	591.5405	2028782	0.00029		2.34125	0
	1:35:42	95.7	2.3925	93.76	0.26758	350.4	208143	0.00168	-0.09832	535.1482	2028782	0.00026		2.3925	0
										2205199		1.08696			

20/80%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	Adj C/Co	M	Mo	M/Mo		pore vol.	CFIT
meth	0:17:35	17.58333	0.439583	4454.08	0.27035	16475.24	194936	0.084516	0.054516	25161.8	1875858	0.013413		0.439583	0
slug	0:19:38	19.63333	0.490833	4836.74	0.26027	18583.55	194936	0.095332	0.065332	28381.72	1875858	0.01513		0.490833	0
	0:21:41	21.68333	0.542083	4745.58	0.27941	16984.29	194936	0.087128	0.057128	25939.25	1875858	0.013828		0.542083	0
flow	0:23:44	23.73333	0.593333	4114.73	0.30475	13501.99	194936	0.069264	0.039264	20620.91	1875858	0.010993		0.593333	0
0.745	0:25:47	25.78333	0.644583	2983.67	0.25697	11610.97	194936	0.059563	0.029563	17732.85	1875858	0.009453		0.644583	0
(mL/min)	0:27:50	27.83333	0.695833	2738.25	0.2808	9751.603	194936	0.050025	0.020025	14893.14	1875858	0.007939		0.695833	0
	0:29:53	29.88333	0.747083	2443.11	0.29083	8400.475	194936	0.043093	0.013093	12829.62	1875858	0.006839		0.747083	0
	0:31:56	31.93333	0.798333	2324.43	0.29098	7988.281	194936	0.040979	0.010979	12200.1	1875858	0.006504		0:798333	0
	0:33:59	33.98333	0.849583	2109.95	0.28872	7307.945	194936	0.037489	0.007489	11161.06	1875858	0.00595		0.849583	0
	0:36:02	36.03333	0.900833	1965.31	0.26784	7337.627	194936	0.037641	0.007641	11206.39	1875858	0.005974		0.900833	0
	0:38:05	38.08333	0.952083	1671.6	0.24671	6775.566	194936	0.034758	0.004758	10347.98	1875858	0.005516		0.952083	0
	0:40:08	40.13333	1.003333	1710.34	0.26998	6335.062	194936	0.032498	0.002498	9675.223	1875858	0.005158		1.003333	0
	0:42:11	42.18333	1.054583	1768.33	0.2862	6178.651	194936	0.031696	0.001696	9436.345	1875858	0.00503		1.054583	0
	0:44:14	44.23333	1.105833	1887.65	0.30551	6178.685	194936	0.031696	0.001696	9436.396	1875858	0.00503		1.105833	0.001
	0:46:17	46.28333	1.157083	1915.83	0.28615	6695.195	194936	0.034346	0.004346	10225.24	1875858	0.005451		1.157083	0.005
	0:48:20	48.33333	1.208333	2851.36	0.30956	9211.009	194936	0.047251	0.017251	14067.51	1875858	0.007499		1.208333	0.023
	0:50:23	50.38333	1.259583	4477.44	0.25374	17645.78	194936	0.090521	0.060521	26949.52	1875858	0.014367		1.259583	0.074
	0:52:26	52.43333	1.310833	10936.48	0.27914	39179.19	194936	0.200985	0.170985	59836.42	1875858	0.031898		1.310833	0.174
	0:54:29	54.48333	1.362083	16805.85	0.23939	70202.81	194936	0.360133	0.330133	107217.2	1875858	0.057156		1.362083	0.326
	0:56:32	56.53333	1.413333	30119.62	0.27699	108739	194936	0.557819	0.527819	166071.7	1875858	0.088531		1.413333	0.508
	0:58:35	58.58333	1.464583	38010.49	0.26573	143041.8	194936	0.733788	0.703788	218460.5	1875858	0.116459		1.464583	0.683
	1:00:38	60.63333	1.515833	46455.3	0.29129	159481.3	194936	0.818121	0.788121	243567.8	1875858	0.129843		1.515833	0.806
	1:02:41	62.68333	1.567083	39179.64	0.23582	166142.1	194936	0.852291	0.822291	253740.6	1875858	0.135266		1.567083	0.857
	1:04:44	64.73333	1.618333	41194.68	0.26956	152821.9	194936	0.78396	0.75396	233397.3	1875858	0.124422		1.618333	0.823
	1:06:47	66.78333	1.669583	37050.2	0.25161	147252.5	194936	0.755389	0.725389	224891.4	1875858	0.119887		1.669583	0.705
	1:08:50	68.83333	1.720833	32546.08	0.26773	121563.1	194936	0.623605	0.593605	185657.2	1875858	0.098972		1.720833	0.537
	1:10:53	70.88333	1.772083	25788.14	0.29943	86124.1	194936	0.441807	0.411807	131533	1875858	0.070119		1.772083	0.36
	1:12:56	72.93333	1.823333	10689.85	0.26672	40078.92	194936	0.2056	0.1756	61210.53	1875858	0.032631		1.823333	0.212
	1:14:59	74.98333	1.874583	3907.36	0.27791	14059.8	194936	0.072125	0.042125	21472.83	1875858	0.011447		1.874583	0.109
	1:17:02	77.03333	1.925833	1444.33	0.28099	5140.147	194936	0.026368	-0.00363	7850.29	1875858	0.004185		1.925833	0.05
	1:19:05	79.08333	1.977083	721.28	0.24233	2976.437	194936	0.015269	-0.01473	4545.764	1875858	0.002423		1.977083	0.02
	1:21:08	81.13333	2.028333	529.54	0.24083	2198.812	194936	0.01128	-0.01872	3358.136	1875858	0.00179		2.028333	0.007
	1:23:11	83.18333	2.079583	477.04	0.28379	1680.961	194936	0.008623	-0.02138	2567.248	1875858	0.001369		2.079583	0.002
	1:25:14	85.23333	2.130833	372.4	0.27904	1334.576	194936	0.006846	-0.02315	2038.231	1875858	0.001087		2.130833	0.001
	1:27:17	87.28333	2.182083	278.78	0.25094	1110.943	194936	0.005699	-0.0243	1696.687	1875858	0.000904		2.182083	0
	1:29:20	89.33333	2.233333	261.16	0.27466	950.8483	194936	0.004878	-0.02512	1452.183	1875858	0.000774		2.233333	0
	1:31:23	91.38333	2.284583	232.67	0.28134	827.0065	194936	0.004242	-0.02576	1263.046	1875858	0.000673		2.284583	0
	1:33:26	93.43333	2.335833	183.17	0.23985	763.6856	194936	0.003918	-0.02608	1166.339	1875858	0.000622		2.335833	0
	1:35:29	95.48333	2.387083	179.1	0.2583	693.3798	194936	0.003557	-0.02644	1058.964	1875858	0.000565		2.387083	0
	1:37:32	97.53333	2.438333	161.33	0.27979	576.611	194936	0.002958	-0.02704	880.6292	1875858	0.000469		2.438333	0
										2205199		1.175568			

50/50%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	Adj C/Co	M	Mo	M/Mo		pore vol.	CFIT
meth	0:16:15	16.25	0.40625	2364.69	0.28663	8249.974	201759	0.04089	0.00089	12599.77	1991614	0.006326		0.40625	0
slug	0:18:18	18.3	0.4575	2529.82	0.26911	9400.691	201759	0.046594	0.006594	14357.21	1991614	0.007209		0.4575	0
	0:20:21	20.35	0.50875	2969.27	0.26909	11034.49	201759	0.054691	0.014691	16852.42	1991614	0.008462		0.50875	0
flow	0:22:24	22.4	0.56	2950.22	0.25981	11355.3	201759	0.056281	0.016281	17342.38	1991614	0.008708		0.56	0
0.745	0:24:27	24.45	0.61125	2739.26	0.27512	9956.601	201759	0.049349	0.009349	15206.22	1991614	0.007635		0.61125	0
(mL/min)	0:26:30	26.5	0.6625	2409	0.28455	8465.999	201759	0.041961	0.001961	12929.7	1991614	0.006492		0.6625	0
	0:28:33	28.55	0.71375	2042.21	0.28475	7171.94	201759	0.035547	-0.00445	10953.35	1991614	0.0055		0.71375	0
	0:30:36	30.6	0.765	1954.81	0.27844	7020.579	201759	0.034797	-0.0052	10722.18	1991614	0.005384		0.765	0
	0:32:39	32.65	0.81625	1842.34	0.26984	6827.527	201759	0.03384	-0.00616	10427.34	1991614	0.005236		0.81625	0
	0:34:42	34.7	0.8675	2009.9	0.315	6380.635	201759	0.031625	-0.00837	9744.825	1991614	0.004893		0.8675	0
	0:36:45	36.75	0.91875	1677.56	0.26949	6224.943	201759	0.030853	-0.00915	9507.045	1991614	0.004774		0.91875	0
	0:38:48	38.8	0.97	1515.55	0.2818	5378.105	201759	0.026656	-0.01334	8213.711	1991614	0.004124		0.97	0
	0:40:51	40.85	1.02125	1375.44	0.26074	5275.14	201759	0.026146	-0.01385	8056.458	1991614	0.004045		1.02125	0.001
	0:42:54	42.9	1.0725	1608.26	0.29565	5439.743	201759	0.026962	-0.01304	8307.847	1991614	0.004171		1.0725	0.005
	0:44:57	44.95	1.12375	1973.91	0.29873	6607.672	201759	0.03275	-0.00725	10091.57	1991614	0.005067		1.12375	0.018
	0:47:00	47	1.175	3033.58	0.26071	11635.84	201759	0.057672	0.017672	17770.84	1991614	0.008923		1.175	0.052
	0:49:03	49.05	1.22625	7000.35	0.29172	23996.81	201759	0.118938	0.078938	36649.13	1991614	0.018402		1.22625	0.119
	0:51:06	51.1	1.2775	15689.03	0.2912	53877.16	201759	0.267037	0.227037	82283.9	1991614	0.041315		1.2775	0.23
	0:53:09	53.15	1.32875	24200.7	0.27575	87763.19	201759	0.43499	0.39499	134036.3	1991614	0.0673		1.32875	0.371
	0:55:12	55.2	1.38	35330.47	0.27012	130795.5	201759	0.648276	0.608276	199757.4	1991614	0.100299		1.38	0.525
	0:57:15	57.25	1.43125	37955.98	0.24936	152213.6	201759	0.754433	0.714433	232468.2	1991614	0.116724		1.43125	0.664
	0:59:18	59.3	1.4825	42188.05	0.27572	153010.5	201759	0.758382	0.718382	233685.3	1991614	0.117335		1.4825	0.763
	1:01:21	61.35	1.53375	42861.35	0.27758	154410.8	201759	0.765323	0.725323	235823.9	1991614	0.118408		1.53375	0.798
	1:03:24	63.4	1.585	41323.98	0.27144	152239.8	201759	0.754563	0.714563	232508.3	1991614	0.116744		1.585	0.763
	1:05:27	65.45	1.63625	41121.33	0.2832	145202.4	201759	0.719683	0.679683	221760.4	1991614	0.111347		1.63625	0.667
	1:07:30	67.5	1.6875	32974.48	0.25616	128726.1	201759	0.638019	0.598019	196596.9	1991614	0.098712		1.6875	0.529
	1:09:33	69.55	1.73875	27193.33	0.26041	104425.1	201759	0.517573	0.477573	159483.2	1991614	0.080077		1.73875	0.383
	1:11:36	71.6	1.79	14820.36	0.24022	61694.95	201759	0.305785	0.265785	94223.61	1991614	0.04731		1.79	0.253
	1:13:39	73.65	1.84125	6962.68	0.25181	27650.53	201759	0.137047	0.097047	42229.27	1991614	0.021204		1.84125	0.153
	1:15:42	75.7	1.8925	3175.93	0.26964	11778.41	201759	0.058379	0.018379	17988.57	1991614	0.009032		1.8925	0.084
	1:17:45	77.75	1.94375	1546.22	0.24612	6282.383	201759	0.031138	-0.00886	9594.769	1991614	0.004818		1.94375	0.043
	1:19:48	79.8	1.995	1048.95	0.26105	4018.196	201759	0.019916	-0.02008	6136.789	1991614	0.003081		1.995	0.02
	1:21:51	81.85	2.04625	733.27	0.25911	2829.956	201759	0.014026	-0.02597	4322.051	1991614	0.00217		2.04625	0.009
	1:23:54	83.9	2.0975	558.25	0.26328	2120.366	201759	0.010509	-0.02949	3238.329	1991614	0.001626		2.0975	0.004
	1:25:57	85.95	2.14875	430.55	0.2525	1705.149	201759	0.008451	-0.03155	2604.188	1991614	0.001308		2.14875	0.001
	1:28:00	88	2.2	394.57	0.26412	1493.904	201759	0.007404	-0.0326	2281.565	1991614	0.001146		2.2	0.001
	1:30:03	90.05	2.25125	349.32	0.26394	1323.483	201759	0.00656	-0.03344	2021.289	1991614	0.001015		2.25125	0
	1:32:06	92.1	2.3025	295.81	0.25511	1159.539	201759	0.005747	-0.03425	1770.906	1991614	0.000889		2.3025	0
	1:34:09	94.15	2.35375	270.49	0.26514	1020.178	201759	0.005056	-0.03494	1558.067	1991614	0.000782		2.35375	0
	1:36:12	96.2	2.405	237.34	0.24317	976.025	201759	0.004838	-0.03516	1490.634	1991614	0.000748		2.405	0
										2347596		1.178741			

0/100%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	M	Mo	M/Mo		pore vol.	CFIT
pce	0:22:05	22.0833	0.55208	1.58	0.29922	5.2804	312928	1.7E-05	8.06448	3100647	2.6E-06		0.55208	0
tracer	0:24:08	24.1333	0.60333	1.62	0.31203	5.19181	312928	1.7E-05	7.92919	3100647	2.6E-06		0.60333	0
	0:26:11	26.1833	0.65458	2.55	0.34117	7.47428	312928	2.4E-05	11.4151	3100647	3.7E-06		0.65458	0
flow	0:28:14	28.2333	0.70583	1.22	0.31864	3.82877	312928	1.2E-05	5.84749	3100647	1.9E-06		0.70583	0
0.745	0:30:17	30.2833	0.75708	1.24	0.29294	4.23295	312928	1.4E-05	6.46477	3100647	2.1E-06		0.75708	0
(mL/min)	0:32:20	32.3333	0.80833	3.42	0.21302	16.0548	312928	5.1E-05	24.5197	3100647	7.9E-06		0.80833	0
	0:34:23	34.3833	0.85958	2.19	0.25764	8.50023	312928	2.7E-05	12.982	3100647	4.2E-06		0.85958	0.001
	0:36:26	36.4333	0.91083	7.83	0.25761	30.3948	312928	9.7E-05	46.4204	3100647	1.5E-05		0.91083	0.007
	0:38:29	38.4833	0.96208	47.2	0.29477	160.125	312928	0.00051	244.551	3100647	7.9E-05		0.96208	0.025
	0:40:32	40.5333	1.01333	166.42	0.25354	656.386	312928	0.0021	1002.46	3100647	0.00032		1.01333	0.067
	0:42:35	42.5833	1.06458	514.08	0.19449	2643.22	312928	0.00845	4036.86	3100647	0.0013		1.06458	0.147
	0:44:38	44.6333	1.11583	5644.13	0.30219	18677.4	312928	0.05969	28525.1	3100647	0.0092		1.11583	0.264
	0:46:41	46.6833	1.16708	25757.7	0.28488	90415.8	312928	0.28893	138088	3100647	0.04454		1.16708	0.408
	0:48:44	48.7333	1.21833	47379.4	0.25282	187404	312928	0.59887	286212	3100647	0.09231		1.21833	0.557
	0:50:47	50.7833	1.26958	60604	0.23892	253658	312928	0.8106	387400	3100647	0.12494		1.26958	0.686
	0:52:50	52.8333	1.32083	78574.5	0.27504	285684	312928	0.91294	436311	3100647	0.14072		1.32083	0.768
	0:54:53	54.8833	1.37208	79118.9	0.26643	296959	312928	0.94897	453531	3100647	0.14627		1.37208	0.788
	0:56:56	56.9333	1.42333	84891.9	0.29374	289004	312928	0.92355	441381	3100647	0.14235		1.42333	0.741
	0:58:59	58.9833	1.47458	60228.6	0.25985	231782	312928	0.74069	353989	3100647	0.11417		1.47458	0.637
	1:01:02	61.0333	1.52583	40149.2	0.27298	147077	312928	0.47	224624	3100647	0.07244		1.52583	0.502
	1:03:05	63.0833	1.57708	22348.6	0.29799	74997.9	312928	0.23966	114541	3100647	0.03694		1.57708	0.363
	1:05:08	65.1333	1.62833	9608.05	0.2612	36784.3	312928	0.11755	56178.8	3100647	0.01812		1.62833	0.242
	1:07:11	67.1833	1.67958	4556.66	0.27898	16333.3	312928	0.0522	24945	3100647	0.00805		1.67958	0.147
	1:09:14	69.2333	1.73083	2170.69	0.2657	8169.7	312928	0.02611	12477.2	3100647	0.00402		1.73083	0.084
	1:11:17	71.2833	1.78208	1464.84	0.29216	5013.83	312928	0.01602	7657.37	3100647	0.00247		1.78208	0.044
	1:13:20	73.3333	1.83333	1365.88	0.35375	3861.14	312928	0.01234	5896.93	3100647	0.0019		1.83333	0.022
	1:15:23	75.3833	1.88458	950.79	0.295	3223.02	312928	0.0103	4922.35	3100647	0.00159		1.88458	0.01
	1:17:26	77.4333	1.93583	768.2	0.27559	2787.47	312928	0.00891	4257.17	3100647	0.00137		1.93583	0.005
	1:19:29	79.4833	1.98708	831.4	0.34071	2440.2	312928	0.0078	3726.79	3100647	0.0012		1.98708	0.002
	1:21:32	81.5333	2.03833	593.07	0.28347	2092.18	312928	0.00669	3195.28	3100647	0.00103		2.03833	0.001
	1:23:35	83.5833	2.08958	477.54	0.26393	1809.34	312928	0.00578	2763.32	3100647	0.00089		2.08958	0
	1:25:38	85.6333	2.14083	468.82	0.31449	1490.73	312928	0.00476	2276.72	3100647	0.00073		2.14083	0
	1:27:41	87.6833	2.19208	326.98	0.28926	1130.4	312928	0.00361	1726.41	3100647	0.00056		2.19208	0
	1:29:44	89.7333	2.24333	265.43	0.30299	876.036	312928	0.0028	1337.93	3100647	0.00043		2.24333	0
	1:31:47	91.7833	2.29458	223.11	0.32482	686.873	312928	0.00219	1049.03	3100647	0.00034		2.29458	0
	1:33:50	93.8333	2.34583	156.13	0.29126	536.05	312928	0.00171	818.683	3100647	0.00026		2.34583	0
	1:35:53	95.8833	2.39708	128.38	0.30931	415.053	312928	0.00133	633.889	3100647	0.0002		2.39708	0
	1:37:56	97.9333	2.44833	92.72	0.26523	349.583	312928	0.00112	533.901	3100647	0.00017		2.44833	0
	1:39:59	99.9833	2.49958	84.69	0.27667	306.105	312928	0.00098	467.498	3100647	0.00015		2.49958	0
	1:42:02	102.033	2.55083	76.42	0.29163	262.044	312928	0.00084	400.207	3100647	0.00013		2.55083	0
									3005273		0.96924			

1/99%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	M	Mo	M/Mo		pore vol.	CFIT
pce	0:20:10	20.16667	0.504167	6.23	0.2993	20.81524	300088	6.94E-05	31.79007	3018135	1.05E-05		0.504167	0
mobil.	0:22:13	22.21667	0.555417	13.5	0.32692	41.29451	300088	0.000138	63.06703	3018135	2.09E-05		0.555417	0
	0:24:16	24.26667	0.606667	41.95	0.30077	139.4753	300088	0.000465	213.0137	3018135	7.06E-05		0.606667	0
flow	0:26:19	26.31667	0.657917	110.61	0.28692	385.5082	300088	0.001285	588.7673	3018135	0.000195		0.657917	0
0.745	0:28:22	28.36667	0.709167	274.83	0.32678	841.0245	300088	0.002803	1284.455	3018135	0.000426		0.709167	0
(mL/min)	0:30:25	30.41667	0.760417	522.43	0.30691	1702.225	300088	0.005672	2599.724	3018135	0.000861		0.760417	0
	0:32:28	32.46667	0.811667	861.5	0.29139	2956.519	300088	0.009852	4515.343	3018135	0.001496		0.811667	0
	0:34:31	34.51667	0.862917	1556.16	0.31419	4952.927	300088	0.016505	7564.357	3018135	0.002506		0.862917	0.001
	0:36:34	36.56667	0.914167	2229.99	0.3014	7398.772	300088	0.024655	11299.78	3018135	0.003744		0.914167	0.005
	0:38:37	38.61667	0.965417	3410.41	0.31696	10759.75	300088	0.035855	16432.83	3018135	0.005445		0.965417	0.019
	0:40:40	40.66667	1.016667	4963.57	0.31184	15917.04	300088	0.053041	24309.3	3018135	0.008054		1.016667	0.055
	0:42:43	42.71667	1.067917	7178.51	0.29156	24621.04	300088	0.082046	37602.48	3018135	0.012459		1.067917	0.121
	0:44:46	44.76667	1.119167	12928.73	0.30482	42414.31	300088	0.14134	64777.26	3018135	0.021463		1.119167	0.223
	0:46:49	46.81667	1.170417	23342.52	0.29452	79256.15	300088	0.26411	121043.9	3018135	0.040106		1.170417	0.355
	0:48:52	48.86667	1.221667	40322.63	0.30067	134109.3	300088	0.4469	204818.4	3018135	0.067863		1.221667	0.502
	0:50:55	50.91667	1.272917	61946.39	0.31707	195371.3	300088	0.651047	298380.9	3018135	0.098863		1.272917	0.634
	0:52:58	52.96667	1.324167	76281.41	0.29659	257194.8	300088	0.857065	392800.8	3018135	0.130147		1.324167	0.732
	0:55:01	55.01667	1.375417	81202.03	0.30404	267076.8	300088	0.889995	407893	3018135	0.135147		1.375417	0.775
	0:57:04	57.06667	1.426667	74733.41	0.28129	265681	300088	0.885344	405761.3	3018135	0.134441		1.426667	0.755
	0:59:07	59.11667	1.477917	72148.01	0.30984	232855.7	300088	0.775958	355628.9	3018135	0.117831		1.477917	0.676
	1:01:10	61.16667	1.529167	61333.12	0.32483	188816.1	300088	0.629202	288369.3	3018135	0.095546		1.529167	0.558
	1:03:13	63.21667	1.580417	40176.09	0.32152	124956.7	300088	0.4164	190840.2	3018135	0.063231		1.580417	0.425
	1:05:16	65.26667	1.631667	18182.75	0.3021	60187.85	300088	0.200567	91921.9	3018135	0.030457		1.631667	0.296
	1:07:19	67.31667	1.682917	5698.56	0.26194	21755.21	300088	0.072496	33225.65	3018135	0.011009		1.682917	0.193
	1:09:22	69.36667	1.734167	2055.15	0.30128	6821.395	300088	0.022731	10417.98	3018135	0.003452		1.734167	0.117
	1:11:25	71.41667	1.785417	903.13	0.28742	3142.196	300088	0.010471	4798.919	3018135	0.00159		1.785417	0.066
	1:13:28	73.46667	1.836667	672.76	0.3089	2177.922	300088	0.007258	3326.231	3018135	0.001102		1.836667	0.035
	1:15:31	75.51667	1.887917	505.23	0.2862	1765.304	300088	0.005883	2696.061	3018135	0.000893		1.887917	0.017
	1:17:34	77.56667	1.939167	492.71	0.31507	1563.811	300088	0.005211	2388.331	3018135	0.000791		1.939167	0.008
	1:19:37	79.61667	1.990417	439.92	0.29212	1505.956	300088	0.005018	2299.972	3018135	0.000762		1.990417	0.004
	1:21:40	81.66667	2.041667	447.6	0.30832	1451.738	300088	0.004838	2217.168	3018135	0.000735		2.041667	0.002
	1:23:43	83.71667	2.092917	464.71	0.32714	1420.523	300088	0.004734	2169.494	3018135	0.000719		2.092917	0.001
	1:25:46	85.76667	2.144167	460.92	0.31857	1446.841	300088	0.004821	2209.687	3018135	0.000732		2.144167	0
	1:27:49	87.81667	2.195417	420.91	0.2827	1488.893	300088	0.004962	2273.912	3018135	0.000753		2.195417	0
	1:29:52	89.86667	2.246667	421.68	0.28468	1481.242	300088	0.004936	2262.227	3018135	0.00075		2.246667	0
	1:31:55	91.91667	2.297917	410.25	0.2835	1447.09	300088	0.004822	2210.068	3018135	0.000732		2.297917	0
	1:33:58	93.96667	2.349167	378.03	0.29724	1271.801	300088	0.004238	1942.357	3018135	0.000644		2.349167	0
	1:36:01	96.01667	2.400417	335.41	0.2904	1154.993	300088	0.003849	1763.963	3018135	0.000584		2.400417	0
	1:38:04	98.06667	2.451667	313.83	0.30426	1031.453	300088	0.003437	1575.287	3018135	0.000522		2.451667	0
	1:40:07	100.1167	2.502917	282.31	0.2999	941.3471	300088	0.003137	1437.672	3018135	0.000476		2.502917	0
									3007956		0.996627			

5/95%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	M	Mo	M/Mo		pore vol.	CFIT
pce	0:24:15	24.25	0.60625	24.28	0.27883	87.07815	336095	0.000259	132.9901	3087318	4.31E-05		0.60625	0
mobil.	0:26:18	26.3	0.6575	76.9	0.31713	242.4873	336095	0.000721	370.3387	3087318	0.00012		0.6575	0
	0:28:21	28.35	0.70875	189.93	0.30453	623.6824	336095	0.001856	952.5189	3087318	0.000309		0.70875	0
flow	0:30:24	30.4	0.76	391.95	0.28275	1386.207	336095	0.004124	2117.084	3087318	0.000686		0.76	0
0.745	0:32:27	32.45	0.81125	831.85	0.32269	2577.861	336095	0.00767	3937.038	3087318	0.001275		0.81125	0
(mL/min)	0:34:30	34.5	0.8625	1239.13	0.27688	4475.332	336095	0.013316	6834.951	3087318	0.002214		0.8625	0
	0:36:33	36.55	0.91375	2406.36	0.32824	7331.099	336095	0.021813	11196.42	3087318	0.003627		0.91375	0
	0:38:36	38.6	0.965	3580.02	0.31534	11352.89	336095	0.033779	17338.7	3087318	0.005616		0.965	0.001
	0:40:39	40.65	1.01625	4886.78	0.29164	16756.21	336095	0.049856	25590.92	3087318	0.008289		1.01625	0.005
	0:42:42	42.7	1.0675	8406.34	0.31856	26388.56	336095	0.078515	40301.93	3087318	0.013054		1.0675	0.025
	0:44:45	44.75	1.11875	13521.76	0.29005	46618.72	336095	0.138707	71198.44	3087318	0.023062		1.11875	0.083
	0:46:48	46.8	1.17	20467.4	0.27096	75536.61	336095	0.224748	115363.3	3087318	0.037367		1.17	0.202
	0:48:51	48.85	1.22125	34138	0.29446	115934.3	336095	0.344945	177060.6	3087318	0.057351		1.22125	0.379
	0:50:54	50.9	1.2725	47216.34	0.27894	169270.6	336095	0.503639	258518.5	3087318	0.083736		1.2725	0.582
	0:52:57	52.95	1.32375	74287.86	0.31499	235842	336095	0.701712	360189.6	3087318	0.116667		1.32375	0.752
	0:55:00	55	1.375	82118.73	0.29904	274607.8	336095	0.817054	419394.8	3087318	0.135844		1.375	0.854
	0:57:03	57.05	1.42625	69263.98	0.24783	279481.8	336095	0.831556	426838.6	3087318	0.138255		1.42625	0.867
	0:59:06	59.1	1.4775	75311.37	0.28515	264111.4	336095	0.785824	403364.2	3087318	0.130652		1.4775	0.781
	1:01:09	61.15	1.52875	53456.32	0.245	218189.1	336095	0.649189	333229.2	3087318	0.107935		1.52875	0.618
	1:03:12	63.2	1.58	36521.73	0.27464	132980.4	336095	0.395663	203094.3	3087318	0.065783		1.58	0.423
	1:05:15	65.25	1.63125	17111.88	0.30742	55662.87	336095	0.165616	85011.12	3087318	0.027536		1.63125	0.249
	1:07:18	67.3	1.6825	5177.87	0.29538	17529.52	336095	0.052156	26771.96	3087318	0.008672		1.6825	0.124
	1:09:21	69.35	1.73375	1895.02	0.28263	6704.95	336095	0.01995	10240.13	3087318	0.003317		1.73375	0.054
	1:11:24	71.4	1.785	1087.8	0.29733	3658.561	336095	0.010885	5587.538	3087318	0.00181		1.785	0.021
	1:13:27	73.45	1.83625	689.68	0.29112	2369.057	336095	0.007049	3618.143	3087318	0.001172		1.83625	0.007
	1:15:30	75.5	1.8875	562.86	0.30316	1856.643	336095	0.005524	2835.559	3087318	0.000918		1.8875	0.002
	1:17:33	77.55	1.93875	470.63	0.29837	1577.337	336095	0.004693	2408.988	3087318	0.00078		1.93875	0.001
	1:19:36	79.6	1.99	419.41	0.30442	1377.735	336095	0.004099	2104.145	3087318	0.000682		1.99	0
	1:21:39	81.65	2.04125	387.44	0.30309	1278.3	336095	0.003803	1952.284	3087318	0.000632		2.04125	0
	1:23:42	83.7	2.0925	368.09	0.30218	1218.115	336095	0.003624	1860.366	3087318	0.000603		2.0925	0
	1:25:45	85.75	2.14375	316.3	0.27866	1135.075	336095	0.003377	1733.543	3087318	0.000562		2.14375	0
	1:27:48	87.8	2.195	319.53	0.29993	1065.349	336095	0.00317	1627.054	3087318	0.000527		2.195	0
	1:29:51	89.85	2.24625	312.82	0.3021	1035.485	336095	0.003081	1581.444	3087318	0.000512		2.24625	0
	1:31:54	91.9	2.2975	290.62	0.2975	976.8739	336095	0.002907	1491.931	3087318	0.000483		2.2975	0
	1:33:57	93.95	2.34875	283.43	0.29978	945.46	336095	0.002813	1443.954	3087318	0.000468		2.34875	0
	1:36:00	96	2.4	260.05	0.28789	903.2964	336095	0.002688	1379.559	3087318	0.000447		2.4	0
	1:38:03	98.05	2.45125	277.52	0.31231	888.6043	336095	0.002644	1357.121	3087318	0.00044		2.45125	0
	1:40:06	100.1	2.5025	252.21	0.28273	892.0525	336095	0.002654	1362.387	3087318	0.000441		2.5025	0
	1:42:09	102.15	2.55375	248.98	0.29302	849.7031	336095	0.002528	1297.709	3087318	0.00042		2.55375	0
	1:44:12	104.2	2.605	222.53	0.28211	788.8058	336095	0.002347	1204.704	3087318	0.00039		2.605	0
									3033894		0.982696			

10/90%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	M	Mo	M/Mo		pore vol.	CFIT
pce	0:18:00	18	0.45	20.82	0.312	66.73077	330477	0.000202	101.9146	3158815	3.23E-05		0.45	0
mobil.	0:20:03	20.05	0.50125	66.1	0.28055	235.6086	330477	0.000713	359.8333	3158815	0.000114		0.50125	0
	0:22:06	22.1	0.5525	180.07	0.29523	609.9312	330477	0.001846	931.5175	3158815	0.000295		0.5525	0
flow	0:24:09	24.15	0.60375	414.97	0.28286	1467.051	330477	0.004439	2240.553	3158815	0.000709		0.60375	0
0.745	0:26:12	26.2	0.655	712.75	0.27981	2547.264	330477	0.007708	3890.309	3158815	0.001232		0.655	0
(mL/min)	0:28:15	28.25	0.70625	1204.84	0.29849	4036.45	330477	0.012214	6164.668	3158815	0.001952		0.70625	0
	0:30:18	30.3	0.7575	1825.59	0.3048	5989.469	330477	0.018124	9147.416	3158815	0.002896		0.7575	0
	0:32:21	32.35	0.80875	2378.39	0.29789	7984.122	330477	0.024159	12193.75	3158815	0.00386		0.80875	0
	0:34:24	34.4	0.86	3200.63	0.29549	10831.6	330477	0.032776	16542.56	3158815	0.005237		0.86	0
	0:36:27	36.45	0.91125	3908.43	0.29122	13420.88	330477	0.040611	20497.05	3158815	0.006489		0.91125	0
	0:38:30	38.5	0.9625	5288.54	0.31541	16767.19	330477	0.050736	25607.69	3158815	0.008107		0.9625	0.001
	0:40:33	40.55	1.01375	6594.05	0.30275	21780.51	330477	0.065906	33264.29	3158815	0.010531		1.01375	0.007
	0:42:36	42.6	1.065	8986.83	0.29121	30860.31	330477	0.093381	47131.4	3158815	0.014921		1.065	0.03
	0:44:39	44.65	1.11625	14676.4	0.29163	50325.41	330477	0.152281	76859.49	3158815	0.024332		1.11625	0.093
	0:46:42	46.7	1.1675	23135.38	0.30645	75494.8	330477	0.228442	115299.4	3158815	0.036501		1.1675	0.215
	0:48:45	48.75	1.21875	34465.5	0.31956	107853	330477	0.326355	164718.5	3158815	0.052146		1.21875	0.388
	0:50:48	50.8	1.27	48089.36	0.29097	165272.6	330477	0.500103	252412.5	3158815	0.079907		1.27	0.578
	0:52:51	52.85	1.32125	65700.31	0.29191	225070.4	330477	0.681047	343738.8	3158815	0.108819		1.32125	0.741
	0:54:54	54.9	1.3725	83744.12	0.3179	263429.1	330477	0.797118	402322.1	3158815	0.127365		1.3725	0.845
	0:56:57	56.95	1.42375	78543.33	0.29254	268487.5	330477	0.812424	410047.5	3158815	0.129811		1.42375	0.866
	0:59:00	59	1.475	79894.62	0.32219	247973.6	330477	0.750351	378717.7	3158815	0.119892		1.475	0.796
	1:01:03	61.05	1.52625	57778.29	0.26668	216657.8	330477	0.655591	330890.6	3158815	0.104751		1.52625	0.65
	1:03:06	63.1	1.5775	45634.57	0.29909	152578.1	330477	0.46169	233024.8	3158815	0.07377		1.5775	0.463
	1:05:09	65.15	1.62875	22443.62	0.30594	73359.55	330477	0.221981	112038.4	3158815	0.035468		1.62875	0.289
	1:07:12	67.2	1.68	7169.69	0.30186	23751.71	330477	0.071871	36274.79	3158815	0.011484		1.68	0.158
	1:09:15	69.25	1.73125	2541	0.2887	8801.524	330477	0.026633	13442.13	3158815	0.004255		1.73125	0.075
	1:11:18	71.3	1.7825	1389.84	0.30252	4594.209	330477	0.013902	7016.505	3158815	0.002221		1.7825	0.031
	1:13:21	73.35	1.83375	860.88	0.27971	3077.759	330477	0.009313	4700.508	3158815	0.001488		1.83375	0.012
	1:15:24	75.4	1.885	658.3	0.293	2246.758	330477	0.006799	3431.361	3158815	0.001086		1.885	0.004
	1:17:27	77.45	1.93625	494.23	0.27682	1785.384	330477	0.005402	2726.728	3158815	0.000863		1.93625	0.001
	1:19:30	79.5	1.9875	426.05	0.28455	1497.276	330477	0.004531	2286.715	3158815	0.000724		1.9875	0
	1:21:33	81.55	2.03875	331.55	0.26365	1257.538	330477	0.003805	1920.576	3158815	0.000608		2.03875	0
	1:23:36	83.6	2.09	335.24	0.3039	1103.126	330477	0.003338	1684.749	3158815	0.000533		2.09	0
	1:25:39	85.65	2.14125	267.85	0.28101	953.1689	330477	0.002884	1455.727	3158815	0.000461		2.14125	0
	1:27:42	87.7	2.1925	249.14	0.28749	866.6041	330477	0.002622	1323.521	3158815	0.000419		2.1925	0
	1:29:45	89.75	2.24375	232.61	0.29245	795.3838	330477	0.002407	1214.75	3158815	0.000385		2.24375	0
	1:31:48	91.8	2.295	207.08	0.28459	727.6433	330477	0.002202	1111.293	3158815	0.000352		2.295	0
	1:33:51	93.85	2.34625	195.4	0.27682	705.8739	330477	0.002136	1078.046	3158815	0.000341		2.34625	0
	1:35:54	95.9	2.3975	186.91	0.27841	671.348	330477	0.002031	1025.316	3158815	0.000325		2.3975	0
	1:37:57	97.95	2.44875	175.27	0.28578	613.3039	330477	0.001856	936.6684	3158815	0.000297		2.44875	0
									3079772		0.974977			

20/80%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	M	Mo	M/Mo		pore vol.	CFIT
pce	0:19:20	19.33333	0.483333	1159.79	0.30853	3759.083	300000	0.01253	5741.06	2793750	0.002055		0.483333	0
mobil.	0:21:23	21.38333	0.534583	1513.23	0.29359	5154.229	300000	0.017181	7871.796	2793750	0.002818		0.534583	0
	0:23:26	23.43333	0.585833	2095.41	0.3165	6620.569	300000	0.022069	10111.26	2793750	0.003619		0.585833	0
flow	0:25:29	25.48333	0.637083	2378.47	0.28774	8266.039	300000	0.027553	12624.31	2793750	0.004519		0.637083	0
0.745	0:27:32	27.53333	0.688333	2676.66	0.27057	9892.671	300000	0.032976	15108.58	2793750	0.005408		0.688333	0
(mL/min)	0:29:35	29.58333	0.739583	3739.89	0.33339	11217.76	300000	0.037393	17132.33	2793750	0.006132		0.739583	0
	0:31:38	31.63333	0.790833	4259.09	0.31983	13316.73	300000	0.044389	20337.98	2793750	0.00728		0.790833	0
	0:33:41	33.68333	0.842083	4358.84	0.28177	15469.5	300000	0.051565	23625.79	2793750	0.008457		0.842083	0
	0:35:44	35.73333	0.893333	5789.58	0.31795	18209.09	300000	0.060697	27809.83	2793750	0.009954		0.893333	0
	0:37:47	37.78333	0.944583	5454.69	0.24726	22060.54	300000	0.073535	33691.97	2793750	0.01206		0.944583	0
	0:39:50	39.83333	0.995833	8374.59	0.3003	27887.41	300000	0.092958	42591.05	2793750	0.015245		0.995833	0.003
	0:41:53	41.88333	1.047083	14147.11	0.31629	44728.29	300000	0.149094	68311.28	2793750	0.024451		1.047083	0.018
	0:43:56	43.93333	1.098333	20908.17	0.30507	68535.65	300000	0.228452	104671.1	2793750	0.037466		1.098333	0.07
	0:45:59	45.98333	1.149583	28003.02	0.29972	93430.6	300000	0.311435	142691.9	2793750	0.051075		1.149583	0.189
	0:48:02	48.03333	1.200833	31910.67	0.29751	107259.2	300000	0.357531	163811.5	2793750	0.058635		1.200833	0.373
	0:50:05	50.08333	1.252083	36777.21	0.25819	142442.4	300000	0.474808	217545.2	2793750	0.077869		1.252083	0.583
	0:52:08	52.13333	1.303333	64668.21	0.32706	197725.8	300000	0.659086	301976.8	2793750	0.10809		1.303333	0.762
	0:54:11	54.18333	1.354583	73093.53	0.29337	249151.3	300000	0.830504	380516.4	2793750	0.136203		1.354583	0.874
	0:56:14	56.23333	1.405833	79287.77	0.30359	261167.3	300000	0.870558	398867.7	2793750	0.142771		1.405833	0.893
	0:58:17	58.28333	1.457083	56759.66	0.2491	227858.9	300000	0.75953	347997.6	2793750	0.124563		1.457083	0.813
	1:00:20	60.33333	1.508333	54031.66	0.27867	193891.2	300000	0.646304	296120.3	2793750	0.105994		1.508333	0.647
	1:02:23	62.38333	1.559583	37734.93	0.2824	133622.3	300000	0.445408	204074.6	2793750	0.073047		1.559583	0.436
	1:04:26	64.43333	1.610833	17971.22	0.26943	66700.89	300000	0.222336	101868.9	2793750	0.036463		1.610833	0.251
	1:06:29	66.48333	1.662083	6774.78	0.28947	23404.08	300000	0.078014	35743.89	2793750	0.012794		1.662083	0.122
	1:08:32	68.53333	1.713333	2783	0.27866	9987.081	300000	0.03329	15252.77	2793750	0.00546		1.713333	0.05
	1:10:35	70.58333	1.764583	1606.5	0.26804	5993.508	300000	0.019978	9153.586	2793750	0.003276		1.764583	0.017
	1:12:38	72.63333	1.815833	1262.35	0.29968	4212.326	300000	0.014041	6433.276	2793750	0.002303		1.815833	0.005
	1:14:41	74.68333	1.867083	935.11	0.27976	3342.544	300000	0.011142	5104.9	2793750	0.001827		1.867083	0.001
	1:16:44	76.73333	1.918333	808.11	0.29278	2760.127	300000	0.0092	4215.404	2793750	0.001509		1.918333	0
	1:18:47	78.78333	1.969583	647.87	0.28958	2237.275	300000	0.007458	3416.878	2793750	0.001223		1.969583	0
	1:20:50	80.83333	2.020833	600.37	0.27606	2174.781	300000	0.007249	3321.434	2793750	0.001189		2.020833	0
	1:22:53	82.88333	2.072083	499.59	0.29517	1692.55	300000	0.005642	2584.947	2793750	0.000925		2.072083	0
	1:24:56	84.93333	2.123333	446.45	0.28542	1564.186	300000	0.005214	2388.903	2793750	0.000855		2.123333	0
	1:26:59	86.98333	2.174583	380.49	0.26874	1415.829	300000	0.004719	2162.325	2793750	0.000774		2.174583	0
	1:29:02	89.03333	2.225833	399.37	0.29257	1365.041	300000	0.00455	2084.759	2793750	0.000746		2.225833	0
	1:31:05	91.08333	2.277083	374.28	0.28596	1308.854	300000	0.004363	1998.948	2793750	0.000716		2.277083	0
	1:33:08	93.13333	2.328333	404.18	0.31267	1292.673	300000	0.004309	1974.235	2793750	0.000707		2.328333	0
	1:35:11	95.18333	2.379583	387.42	0.2906	1333.173	300000	0.004444	2036.088	2793750	0.000729		2.379583	0
	1:37:14	97.23333	2.430833	371.45	0.289	1285.294	300000	0.004284	1962.965	2793750	0.000703		2.430833	0
	1:39:17	99.28333	2.482083	327.79	0.27217	1204.358	300000	0.004015	1839.355	2793750	0.000658		2.482083	0
									3046774		1.090568			

50/50%	time	conv.	pore vol.	dpm	diff	dpm/diff	Co	C/Co	M	Mo	M/Mo		pore vol.	CFIT
pce	0:17:20	17.33333	0.433333	874.28	0.30698	2848.003	340533	0.008363	4349.613	3298062	0.001319		0.433333	0
mobil.	0:19:23	19.38333	0.484583	1315.54	0.28404	4631.531	340533	0.013601	7073.505	3298062	0.002145		0.484583	0
	0:21:26	21.43333	0.535833	1896.97	0.29132	6511.637	340533	0.019122	9944.897	3298062	0.003015		0.535833	0
flow	0:23:29	23.48333	0.587083	2363.15	0.29264	8075.28	340533	0.023714	12332.97	3298062	0.003739		0.587083	0
0.745	0:25:32	25.53333	0.638333	2859.65	0.28363	10082.33	340533	0.029607	15398.23	3298062	0.004669		0.638333	0
(mL/min)	0:27:35	27.58333	0.689583	2931.23	0.24484	11972.02	340533	0.035157	18284.27	3298062	0.005544		0.689583	0
	0:29:38	29.63333	0.740833	4133.06	0.31632	13066.07	340533	0.038369	19955.16	3298062	0.006051		0.740833	0
	0:31:41	31.68333	0.792083	4081.07	0.26427	15442.8	340533	0.045349	23585.02	3298062	0.007151		0.792083	0
	0:33:44	33.73333	0.843333	5179.37	0.29769	17398.54	340533	0.051092	26571.91	3298062	0.008057		0.843333	0
	0:35:47	35.78333	0.894583	5323.75	0.20651	25779.62	340533	0.075704	39371.93	3298062	0.011938		0.894583	0
	0:37:50	37.83333	0.945833	6887.87	0.29388	23437.7	340533	0.068827	35795.22	3298062	0.010853		0.945833	0.002
	0:39:53	39.88333	0.997083	8218.45	0.26754	30718.58	340533	0.090207	46914.96	3298062	0.014225		0.997083	0.011
	0:41:56	41.93333	1.048333	12478.23	0.28221	44216.12	340533	0.129844	67529.06	3298062	0.020475		1.048333	0.038
	0:43:59	43.98333	1.099583	18074.86	0.26325	68660.44	340533	0.201626	104861.7	3298062	0.031795		1.099583	0.103
	0:46:02	46.03333	1.150833	26627.14	0.28533	93320.51	340533	0.274042	142523.7	3298062	0.043214		1.150833	0.215
	0:48:05	48.08333	1.202083	31560.02	0.27632	114215.5	340533	0.335402	174435.6	3298062	0.05289		1.202083	0.37
	0:50:08	50.13333	1.253333	42102.3	0.29584	142314.4	340533	0.417917	217349.7	3298062	0.065902		1.253333	0.541
	0:52:11	52.18333	1.304583	53185	0.26629	199725.9	340533	0.58651	305031.3	3298062	0.092488		1.304583	0.698
	0:54:14	54.23333	1.355833	64220.88	0.23552	272677	340533	0.800736	416445.9	3298062	0.12627		1.355833	0.801
	0:56:17	56.28333	1.407083	80991.62	0.26375	307077.2	340533	0.901755	468983.7	3298062	0.1422		1.407083	0.835
	0:58:20	58.33333	1.458333	81131.92	0.27473	295315.1	340533	0.867214	451020	3298062	0.136753		1.458333	0.788
	1:00:23	60.38333	1.509583	69519.22	0.27891	249253.2	340533	0.73195	380672	3298062	0.115423		1.509583	0.669
	1:02:26	62.43333	1.560833	43099.63	0.2739	157355.3	340533	0.462085	240321	3298062	0.072867		1.560833	0.511
	1:04:29	64.48333	1.612083	20457.33	0.25065	81617.12	340533	0.239675	124649.7	3298062	0.037795		1.612083	0.349
	1:06:32	66.53333	1.663333	13732.04	0.28036	48980.03	340533	0.143833	74804.74	3298062	0.022681		1.663333	0.214
	1:08:35	68.58333	1.714583	7758.49	0.27171	28554.3	340533	0.083852	43609.56	3298062	0.013223		1.714583	0.116
	1:10:38	70.63333	1.765833	5318.8	0.25223	21087.1	340533	0.061924	32205.28	3298062	0.009765		1.765833	0.058
	1:12:41	72.68333	1.817083	3995.84	0.25598	15609.97	340533	0.04584	23840.33	3298062	0.007229		1.817083	0.026
	1:14:44	74.73333	1.868333	2685.7	0.26295	10213.73	340533	0.029993	15598.92	3298062	0.00473		1.868333	0.011
	1:16:47	76.78333	1.919583	1747.7	0.26904	6496.06	340533	0.019076	9921.108	3298062	0.003008		1.919583	0.004
	1:18:50	78.83333	1.970833	1079.37	0.25912	4165.522	340533	0.012232	6361.793	3298062	0.001929		1.970833	0.001
	1:20:53	80.88333	2.022083	706.88	0.24885	2840.587	340533	0.008342	4338.286	3298062	0.001315		2.022083	0
	1:22:56	82.93333	2.073333	530.9	0.27477	1932.161	340533	0.005674	2950.894	3298062	0.000895		2.073333	0
	1:24:59	84.98333	2.124583	436.45	0.26683	1635.686	340533	0.004803	2498.101	3298062	0.000757		2.124583	0
	1:27:02	87.03333	2.175833	343.78	0.25692	1338.082	340533	0.003929	2043.586	3298062	0.00062		2.175833	0
	1:29:05	89.08333	2.227083	304.76	0.2656	1147.44	340533	0.00337	1752.427	3298062	0.000531		2.227083	0
	1:31:08	91.13333	2.278333	263.51	0.25724	1024.374	340533	0.003008	1564.475	3298062	0.000474		2.278333	0
	1:33:11	93.18333	2.329583	215.32	0.24725	870.8595	340533	0.002557	1330.02	3298062	0.000403		2.329583	0
	1:35:14	95.23333	2.380833	204.73	0.24934	821.0877	340533	0.002411	1254.006	3298062	0.00038		2.380833	0
	1:37:17	97.28333	2.432083	189.36	0.25113	754.0318	340533	0.002214	1151.595	3298062	0.000349		2.432083	0
									3578626		1.085069			

Appendix B. CFITM Input Files

```
    1
    2    1   25  40
  Methanol Run: 0% Methanol/100% Water
PECLET       RF           PULSE
      5.0         1.0      0.319
    1    1    0
     0.400  0.0000
     0.451  0.0000
     0.503  0.0000
     0.554  0.0000
     0.605  0.0000
     0.656  0.0000
     0.708  0.0000
     0.759  0.0000
     0.810  0.0000
     0.861  0.0000
     0.913  0.0000
     0.964  0.0028
     1.015  0.0111
     1.066  0.0184
     1.118  0.0320
     1.169  0.0563
     1.220  0.0911
     1.271  0.1527
     1.323  0.2566
     1.374  0.4205
     1.425  0.5675
     1.476  0.6260
     1.528  0.6289
     1.579  0.5736
     1.630  0.4732
     1.681  0.3275
     1.733  0.1455
     1.784  0.0284
     1.835  0.0000
     1.886  0.0000
     1.938  0.0000
     1.989  0.0000
     2.040  0.0000
     2.091  0.0000
     2.143  0.0000
     2.194  0.0000
     2.245  0.0000
     2.296  0.0000
     2.348  0.0000
     2.399  0.0000
C$stop
```

```
     1
     2    1   25  40
  Methanol Run: 1% Methanol/99% Water
PECLET        RF           PULSE
      5.0         1.0      0.326
     1    1     0
      0.431   0.0000
      0.483   0.0000
      0.534   0.0000
      0.585   0.0000
      0.636   0.0000
      0.688   0.0000
      0.739   0.0000
      0.790   0.0000
      0.841   0.0000
      0.893   0.0000
      0.944   0.0000
      0.995   0.0046
      1.046   0.0136
      1.098   0.0245
      1.149   0.0436
      1.200   0.0820
      1.251   0.1352
      1.303   0.2179
      1.354   0.3383
      1.405   0.4895
      1.456   0.6194
      1.508   0.6339
      1.559   0.6113
      1.610   0.5364
      1.661   0.4029
      1.713   0.2162
      1.764   0.0678
      1.815   0.0000
      1.866   0.0000
      1.918   0.0000
      1.969   0.0000
      2.020   0.0000
      2.071   0.0000
      2.123   0.0000
      2.174   0.0000
      2.225   0.0000
      2.276   0.0000
      2.328   0.0000
      2.379   0.0000
      2.430   0.0000
C$stop
```

```
    1
    2    1    25  40
  Methanol Run: 5% Methanol/95% Water
PECLET        RF           PULSE
      5.0          1.0       0.326
    1    1     0
     0.456  0.0000
     0.508  0.0000
     0.559  0.0000
     0.610  0.0000
     0.661  0.0000
     0.713  0.0000
     0.764  0.0000
     0.815  0.0000
     0.866  0.0000
     0.918  0.0000
     0.969  0.0000
     1.020  0.0000
     1.071  0.0024
     1.123  0.0108
     1.174  0.0318
     1.225  0.0926
     1.276  0.2447
     1.328  0.4720
     1.379  0.6573
     1.430  0.7483
     1.481  0.7455
     1.533  0.7510
     1.584  0.6581
     1.635  0.4568
     1.686  0.1993
     1.738  0.0302
     1.789  0.0000
     1.840  0.0000
     1.891  0.0000
     1.943  0.0000
     1.994  0.0000
     2.045  0.0000
     2.096  0.0000
     2.148  0.0000
     2.199  0.0000
     2.250  0.0000
     2.301  0.0000
     2.353  0.0000
     2.404  0.0000
     2.455  0.0000
C$stop
```

```
     1
     2   . 1    25  40
   Methanol Run: 10% Methanol/90% Water
 PECLET       RF          PULSE
       5.0         1.0      0.328
     1    1     0
      0.394   0.0000
      0.445   0.0000
      0.496   0.0000
      0.548   0.0000
      0.599   0.0000
      0.650   0.0000
      0.701   0.0000
      0.753   0.0000
      0.804   0.0000
      0.855   0.0000
      0.906   0.0000
      0.958   0.0000
      1.009   0.0000
      1.060   0.0018
      1.111   0.0041
      1.163   0.0353
      1.214   0.1728
      1.265   0.4012
      1.316   0.6129
      1.368   0.7223
      1.419   0.8058
      1.470   0.7435
      1.521   0.6161
      1.573   0.5071
      1.624   0.3088
      1.675   0.0880
      1.726   0.0000
      1.778   0.0000
      1.829   0.0000
      1.880   0.0000
      1.931   0.0000
      1.983   0.0000
      2.034   0.0000
      2.085   0.0000
      2.136   0.0000
      2.188   0.0000
      2.239   0.0000
      2.290   0.0000
      2.341   0.0000
      2.393   0.0000
C$stop
```

```
     1
     2    .1    25   40
  Methanol Run: 20% Methanol/80% Water
PECLET         RF            PULSE
       5.0          1.0       0.322
     1     1      0
      0.440   0.0000
      0.491   0.0000
      0.542   0.0000
      0.593   0.0000
      0.645   0.0000
      0.696   0.0000
      0.747   0.0000
      0.798   0.0000
      0.850   0.0000
      0.901   0.0000
      0.952   0.0000
      1.003   0.0000
      1.055   0.0017
      1.106   0.0017
      1.157   0.0043
      1.208   0.0173
      1.260   0.0605
      1.311   0.1710
      1.362   0.3301
      1.413   0.5278
      1.465   0.7038
      1.516   0.7881
      1.567   0.8223
      1.618   0.7540
      1.670   0.7254
      1.721   0.5936
      1.772   0.4118
      1.823   0.1756
      1.875   0.0421
      1.926   0.0000
      1.977   0.0000
      2.028   0.0000
      2.080   0.0000
      2.131   0.0000
      2.182   0.0000
      2.233   0.0000
      2.285   0.0000
      2.336   0.0000
      2.387   0.0000
      2.438   0.0000
C$stop
```

```
     1
     2   . 1    25  40
  Methanol Run: 50% Methanol/50% Water
PECLET        RF            PULSE
      5.0         1.0      0.331
     1    1     0
      0.406  0.0000
      0.458  0.0000
      0.509  0.0000
      0.560  0.0000
      0.611  0.0000
      0.663  0.0000
      0.714  0.0000
      0.765  0.0000
      0.816  0.0000
      0.868  0.0000
      0.919  0.0000
      0.970  0.0000
      1.021  0.0000
      1.073  0.0000
      1.124  0.0000
      1.175  0.0177
      1.226  0.0789
      1.278  0.2270
      1.329  0.3950
      1.380  0.6083
      1.431  0.7144
      1.483  0.7184
      1.534  0.7253
      1.585  0.7146
      1.636  0.6797
      1.688  0.5980
      1.739  0.4776
      1.790  0.2658
      1.841  0.0970
      1.893  0.0184
      1.944  0.0000
      1.995  0.0000
      2.046  0.0000
      2.098  0.0000
      2.149  0.0000
      2.200  0.0000
      2.251  0.0000
      2.303  0.0000
      2.354  0.0000
      2.405  0.0000
C$stop
```

```
     1
     2    .1    25   40
   PCE Run:  0% Methanol/100% Water
 PECLET        RF           PULSE
     159.          1.0       0.334
     0     1     0     0     0
      0.552   0.0000
      0.603   0.0000
      0.655   0.0000
      0.706   0.0000
      0.757   0.0000
      0.808   0.0000
      0.860   0.0000
      0.911   0.0000
      0.962   0.0005
      1.013   0.0021
      1.065   0.0084
      1.116   0.0597
      1.167   0.2889
      1.218   0.5989
      1.270   0.8106
      1.321   0.9129
      1.372   0.9490
      1.423   0.9235
      1.475   0.7407
      1.526   0.4700
      1.577   0.2397
      1.628   0.1175
      1.680   0.0521
      1.731   0.0261
      1.782   0.0160
      1.833   0.0123
      1.885   0.0103
      1.936   0.0089
      1.987   0.0078
      2.038   0.0067
      2.090   0.0058
      2.141   0.0048
      2.192   0.0036
      2.243   0.0028
      2.295   0.0022
      2.346   0.0017
      2.397   0.0013
      2.448   0.0011
      2.500   0.0010
      2.551   0.0008
C$stop
```

```
     1
     2    1   25  40
   PCE Run: 1% Methanol/99% Water
 PECLET       RF           PULSE
     153.          1.0      0.337
     0    1    0
      0.504  0.0000
      0.555  0.0001
      0.607  0.0005
      0.658  0.0013
      0.709  0.0028
      0.760  0.0057
      0.812  0.0099
      0.863  0.0165
      0.914  0.0247
      0.965  0.0359
      1.017  0.0530
      1.068  0.0820
      1.119  0.1413
      1.170  0.2641
      1.222  0.4469
      1.273  0.6510
      1.324  0.8571
      1.375  0.8900
      1.427  0.8853
      1.478  0.7760
      1.529  0.6292
      1.580  0.4164
      1.632  0.2006
      1.683  0.0725
      1.734  0.0227
      1.785  0.0105
      1.837  0.0073
      1.888  0.0059
      1.939  0.0052
      1.990  0.0050
      2.042  0.0048
      2.093  0.0047
      2.144  0.0048
      2.195  0.0050
      2.247  0.0049
      2.298  0.0048
      2.349  0.0042
      2.400  0.0038
      2.452  0.0034
      2.503  0.0031
C$stop
```

```
     1
     2    1   25  40
   PCE Run: 5% Methanol/95% Water
 PECLET       RF          PULSE
     305.         1.0      0.309
     0    1     0
      0.606   0.0003
      0.658   0.0007
      0.709   0.0019
      0.760   0.0041
      0.811   0.0077
      0.863   0.0133
      0.914   0.0218
      0.965   0.0338
      1.016   0.0499
      1.068   0.0785
      1.119   0.1387
      1.170   0.2247
      1.221   0.3449
      1.273   0.5036
      1.324   0.7017
      1.375   0.8171
      1.426   0.8316
      1.478   0.7858
      1.529   0.6491
      1.580   0.3957
      1.631   0.1656
      1.683   0.0522
      1.734   0.0200
      1.785   0.0109
      1.836   0.0070
      1.888   0.0055
      1.939   0.0047
      1.990   0.0041
      2.041   0.0038
      2.093   0.0036
      2.144   0.0034
      2.195   0.0032
      2.246   0.0031
      2.298   0.0029
      2.349   0.0028
      2.400   0.0027
      2.451   0.0026
      2.503   0.0027
      2.554   0.0025
      2.605   0.0023
C$stop
```

```
    1
    2    1    25  40
  PCE Run: 10% Methanol/90% Water
PECLET       RF           PULSE
    276.          1.0      0.320
    0    1     0
     0.450  0.0002
     0.501  0.0007
     0.553  0.0018
     0.604  0.0044
     0.655  0.0077
     0.706  0.0122
     0.758  0.0181
     0.809  0.0242
     0.860  0.0328
     0.911  0.0406
     0.963  0.0507
     1.014  0.0659
     1.065  0.0934
     1.116  0.1523
     1.168  0.2284
     1.219  0.3264
     1.270  0.5001
     1.321  0.6810
     1.373  0.7971
     1.424  0.8124
     1.475  0.7504
     1.526  0.6556
     1.578  0.4617
     1.629  0.2220
     1.680  0.0719
     1.731  0.0266
     1.783  0.0139
     1.834  0.0093
     1.885  0.0068
     1.936  0.0054
     1.988  0.0045
     2.039  0.0038
     2.090  0.0033
     2.141  0.0029
     2.193  0.0026
     2.244  0.0024
     2.295  0.0022
     2.346  0.0021
     2.398  0.0020
     2.449  0.0019
C$stop
```

```
     1
     2    1    25  40
   PCE Run: 20% Methanol/80% Water
 PECLET       RF           PULSE
     328.          1.0      0.313
     0    1     0
      0.483  0.0125
      0.535  0.0172
      0.586  0.0221
      0.637  0.0276
      0.688  0.0330
      0.740  0.0374
      0.791  0.0444
      0.842  0.0516
      0.893  0.0607
      0.945  0.0735
      0.996  0.0930
      1.047  0.1491
      1.098  0.2285
      1.150  0.3114
      1.201  0.3575
      1.252  0.4748
      1.303  0.6591
      1.355  0.8305
      1.406  0.8706
      1.457  0.7595
      1.508  0.6463
      1.560  0.4454
      1.611  0.2223
      1.662  0.0708
      1.713  0.0333
      1.765  0.0120
      1.816  0.0140
      1.867  0.0111
      1.918  0.0092
      1.970  0.0075
      2.021  0.0072
      2.072  0.0056
      2.123  0.0052
      2.175  0.0047
      2.226  0.0046
      2.277  0.0044
      2.328  0.0043
      2.380  0.0044
      2.431  0.0043
      2.482  0.0040
C$stop
```

```
    1
    2    1   25  40
  PCE Run: 50% Methanol/50% Water
PECLET       RF          PULSE
    221.         1.0      0.326
    0    1    0
     0.433  0.0084
     0.485  0.0136
     0.536  0.0191
     0.587  0.0237
     0.638  0.0296
     0.690  0.0352
     0.741  0.0384
     0.792  0.0453
     0.843  0.0511
     0.895  0.0757
     0.946  0.0688
     0.997  0.0902
     1.048  0.1298
     1.100  0.2016
     1.151  0.2740
     1.202  0.3354
     1.253  0.4179
     1.305  0.5865
     1.356  0.8007
     1.407  0.9018
     1.458  0.8672
     1.510  0.7320
     1.561  0.4621
     1.612  0.2397
     1.663  0.1438
     1.715  0.0839
     1.766  0.0619
     1.817  0.0458
     1.868  0.0300
     1.920  0.0191
     1.971  0.0122
     2.022  0.0083
     2.073  0.0057
     2.125  0.0048
     2.176  0.0039
     2.227  0.0034
     2.278  0.0030
     2.330  0.0026
     2.381  0.0024
     2.432  0.0022
C$stop
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Appendix C. CFITM Output Files

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 0% Methanol/100% Water

****

INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	5.000
2	RF	1.000
3	PUL	0.319

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4000	0.0000
2	0.4510	0.0000
3	0.5030	0.0000
4	0.5540	0.0000
5	0.6050	0.0000
6	0.6560	0.0000
7	0.7080	0.0000
8	0.7590	0.0000
9	0.8100	0.0000
10	0.8610	0.0000
11	0.9130	0.0000
12	0.9640	0.0028
13	1.0150	0.0111
14	1.0660	0.0184
15	1.1180	0.0320
16	1.1690	0.0563
17	1.2200	0.0911
18	1.2710	0.1527
19	1.3230	0.2566
20	1.3740	0.4205
21	1.4250	0.5675
22	1.4760	0.6260
23	1.5280	0.6289
24	1.5790	0.5736
25	1.6300	0.4732
26	1.6810	0.3275
27	1.7330	0.1455
28	1.7840	0.0284
29	1.8350	0.0000
30	1.8860	0.0000
31	1.9380	0.0000
32	1.9890	0.0000
33	2.0400	0.0000
34	2.0910	0.0000
35	2.1430	0.0000
36	2.1940	0.0000
37	2.2450	0.0000
38	2.2960	0.0000

39	2.3480	0.0000
40	2.3990	0.0000

ITERATION	SSQ	PECLET	RF
0	1.7375172	5.00000	1.00000
1	1.3608561	3.95501	1.61202
2	1.1148545	10.48430	1.57499
3	0.9179355	21.69042	1.26549
4	0.6162016	39.98299	1.41942
5	0.4030838	66.54190	1.31392
6	0.2705094	100.95358	1.35637
7	0.2326818	130.64368	1.34381
8	0.2254175	148.79398	1.34595
9	0.2245778	156.06346	1.34598
10	0.2245075	158.40369	1.34605
11	0.2245041	159.08281	1.34607
12	0.2245041	159.09472	1.34607

CORRELATION MATRIX

	1	2
1	1.0000	
2	0.0432	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	PECLET	159.09472	23.1279	6.88	112.2719	205.9175
2	RF	1.34607	0.0110	122.14	1.3238	1.3684

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.400	0.000	0.000	0.000	13	1.015	0.011	0.006	0.005
2	0.451	0.000	0.000	0.000	12	0.964	0.003	0.001	0.001
3	0.503	0.000	0.000	0.000	14	1.066	0.018	0.018	0.000
4	0.554	0.000	0.000	0.000	1	0.400	0.000	0.000	0.000
5	0.605	0.000	0.000	0.000	2	0.451	0.000	0.000	0.000
6	0.656	0.000	0.000	0.000	3	0.503	0.000	0.000	0.000
7	0.708	0.000	0.000	0.000	4	0.554	0.000	0.000	0.000
8	0.759	0.000	0.000	0.000	5	0.605	0.000	0.000	0.000
9	0.810	0.000	0.000	0.000	6	0.656	0.000	0.000	0.000
10	0.861	0.000	0.000	0.000	7	0.708	0.000	0.000	0.000
11	0.913	0.000	0.000	0.000	8	0.759	0.000	0.000	0.000
12	0.964	0.003	0.001	0.001	9	0.810	0.000	0.000	0.000
13	1.015	0.011	0.006	0.005	10	0.861	0.000	0.000	0.000
14	1.066	0.018	0.018	0.000	40	2.399	0.000	0.000	0.000
15	1.118	0.032	0.048	-0.016	39	2.348	0.000	0.000	0.000
16	1.169	0.056	0.103	-0.047	11	0.913	0.000	0.000	0.000
17	1.220	0.091	0.189	-0.098	38	2.296	0.000	0.000	0.000
18	1.271	0.153	0.303	-0.150	37	2.245	0.000	0.001	-0.001
19	1.323	0.257	0.434	-0.178	36	2.194	0.000	0.001	-0.001
20	1.374	0.420	0.558	-0.138	35	2.143	0.000	0.003	-0.003
21	1.425	0.568	0.656	-0.088	34	2.091	0.000	0.007	-0.007
22	1.476	0.626	0.708	-0.082	33	2.040	0.000	0.014	-0.014

23	1.528	0.629	0.704	-0.075	15	1.118	0.032	0.048	-0.016
24	1.579	0.574	0.646	-0.073	32	1.989	0.000	0.026	-0.026
25	1.630	0.473	0.550	-0.077	16	1.169	0.056	0.103	-0.047
26	1.681	0.328	0.435	-0.108	31	1.938	0.000	0.049	-0.049
27	1.733	0.145	0.318	-0.173	24	1.579	0.574	0.646	-0.073
28	1.784	0.028	0.219	-0.190	23	1.528	0.629	0.704	-0.075
29	1.835	0.000	0.141	-0.141	25	1.630	0.473	0.550	-0.077
30	1.886	0.000	0.086	-0.086	22	1.476	0.626	0.708	-0.082
31	1.938	0.000	0.049	-0.049	30	1.886	0.000	0.086	-0.086
32	1.989	0.000	0.026	-0.026	21	1.425	0.568	0.656	-0.088
33	2.040	0.000	0.014	-0.014	17	1.220	0.091	0.189	-0.098
34	2.091	0.000	0.007	-0.007	26	1.681	0.328	0.435	-0.108
35	2.143	0.000	0.003	-0.003	20	1.374	0.420	0.558	-0.138
36	2.194	0.000	0.001	-0.001	29	1.835	0.000	0.141	-0.141
37	2.245	0.000	0.001	-0.001	18	1.271	0.153	0.303	-0.150
38	2.296	0.000	0.000	0.000	27	1.733	0.145	0.318	-0.173
39	2.348	0.000	0.000	0.000	19	1.323	0.257	0.434	-0.178
40	2.399	0.000	0.000	0.000	28	1.784	0.028	0.219	-0.190

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 1% Methanol/99% Water

****

INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	5.000
2	RF	1.000
3	PUL	0.326

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4310	0.0000
2	0.4830	0.0000
3	0.5340	0.0000
4	0.5850	0.0000
5	0.6360	0.0000
6	0.6880	0.0000
7	0.7390	0.0000
8	0.7900	0.0000
9	0.8410	0.0000
10	0.8930	0.0000
11	0.9440	0.0000
12	0.9950	0.0046
13	1.0460	0.0136
14	1.0980	0.0245
15	1.1490	0.0436
16	1.2000	0.0820
17	1.2510	0.1352
18	1.3030	0.2179
19	1.3540	0.3383
20	1.4050	0.4895
21	1.4560	0.6194
22	1.5080	0.6339
23	1.5590	0.6113
24	1.6100	0.5364
25	1.6610	0.4029
26	1.7130	0.2162
27	1.7640	0.0678
28	1.8150	0.0000
29	1.8660	0.0000
30	1.9180	0.0000
31	1.9690	0.0000
32	2.0200	0.0000
33	2.0710	0.0000
34	2.1230	0.0000
35	2.1740	0.0000
36	2.2250	0.0000
37	2.2760	0.0000
38	2.3280	0.0000

39	2.3790	0.0000
40	2.4300	0.0000

ITERATION	SSQ	PECLET	RF
0	1.7593414	5.00000	1.00000
1	1.3673960	4.02193	1.60697
2	1.1304704	10.36198	1.57879
3	0.9330030	20.88302	1.26978
4	0.6351175	38.60093	1.41651
5	0.4244203	63.76383	1.31535
6	0.2966283	96.48217	1.35419
7	0.2591371	124.63864	1.34265
8	0.2515045	142.14987	1.34461
9	0.2505274	149.52063	1.34467
10	0.2504351	152.03288	1.34476
11	0.2504297	152.80571	1.34478
12	0.2504297	152.83439	1.34478

1 CORRELATION MATRIX

	1	2
1	1.0000	
2	0.0425	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	PECLET	152.83439	23.2397	6.58	105.7853	199.8834
2	RF	1.34478	0.0117	114.60	1.3210	1.3685

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.431	0.000	0.000	0.000	12	0.995	0.005	0.004	0.001
2	0.483	0.000	0.000	0.000	13	1.046	0.014	0.014	0.000
3	0.534	0.000	0.000	0.000	1	0.431	0.000	0.000	0.000
4	0.585	0.000	0.000	0.000	2	0.483	0.000	0.000	0.000
5	0.636	0.000	0.000	0.000	3	0.534	0.000	0.000	0.000
6	0.688	0.000	0.000	0.000	4	0.585	0.000	0.000	0.000
7	0.739	0.000	0.000	0.000	5	0.636	0.000	0.000	0.000
8	0.790	0.000	0.000	0.000	6	0.688	0.000	0.000	0.000
9	0.841	0.000	0.000	0.000	7	0.739	0.000	0.000	0.000
10	0.893	0.000	0.000	0.000	8	0.790	0.000	0.000	0.000
11	0.944	0.000	0.001	-0.001	9	0.841	0.000	0.000	0.000
12	0.995	0.005	0.004	0.001	40	2.430	0.000	0.000	0.000
13	1.046	0.014	0.014	0.000	39	2.379	0.000	0.000	0.000
14	1.098	0.025	0.037	-0.013	10	0.893	0.000	0.000	0.000
15	1.149	0.044	0.084	-0.040	38	2.328	0.000	0.000	0.000
16	1.200	0.082	0.159	-0.077	37	2.276	0.000	0.001	-0.001
17	1.251	0.135	0.262	-0.127	11	0.944	0.000	0.001	-0.001
18	1.303	0.218	0.388	-0.170	36	2.225	0.000	0.001	-0.001
19	1.354	0.338	0.515	-0.176	35	2.174	0.000	0.003	-0.003
20	1.405	0.489	0.623	-0.133	34	2.123	0.000	0.005	-0.005
21	1.456	0.619	0.694	-0.074	33	2.071	0.000	0.011	-0.011
22	1.508	0.634	0.714	-0.080	14	1.098	0.025	0.037	-0.013

23	1.559	0.611	0.680	-0.068	32	2.020	0.000	0.021	-0.021
24	1.610	0.536	0.601	-0.064	31	1.969	0.000	0.039	-0.039
25	1.661	0.403	0.494	-0.091	15	1.149	0.044	0.084	-0.040
26	1.713	0.216	0.377	-0.160	24	1.610	0.536	0.601	-0.064
27	1.764	0.068	0.270	-0.202	23	1.559	0.611	0.680	-0.068
28	1.815	0.000	0.182	-0.182	30	1.918	0.000	0.068	-0.068
29	1.866	0.000	0.115	-0.115	21	1.456	0.619	0.694	-0.074
30	1.918	0.000	0.068	-0.068	16	1.200	0.082	0.159	-0.077
31	1.969	0.000	0.039	-0.039	22	1.508	0.634	0.714	-0.080
32	2.020	0.000	0.021	-0.021	25	1.661	0.403	0.494	-0.091
33	2.071	0.000	0.011	-0.011	29	1.866	0.000	0.115	-0.115
34	2.123	0.000	0.005	-0.005	17	1.251	0.135	0.262	-0.127
35	2.174	0.000	0.003	-0.003	20	1.405	0.489	0.623	-0.133
36	2.225	0.000	0.001	-0.001	26	1.713	0.216	0.377	-0.160
37	2.276	0.000	0.001	-0.001	18	1.303	0.218	0.388	-0.170
38	2.328	0.000	0.000	0.000	19	1.354	0.338	0.515	-0.176
39	2.379	0.000	0.000	0.000	28	1.815	0.000	0.182	-0.182
40	2.430	0.000	0.000	0.000	27	1.764	0.068	0.270	-0.202

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 5% Methanol/95% Water

****

INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	5.000
2	RF	1.000
3	PUL	0.326

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4560	0.0000
2	0.5080	0.0000
3	0.5590	0.0000
4	0.6100	0.0000
5	0.6610	0.0000
6	0.7130	0.0000
7	0.7640	0.0000
8	0.8150	0.0000
9	0.8660	0.0000
10	0.9180	0.0000
11	0.9690	0.0000
12	1.0200	0.0000
13	1.0710	0.0024
14	1.1230	0.0108
15	1.1740	0.0318
16	1.2250	0.0926
17	1.2760	0.2447
18	1.3280	0.4720
19	1.3790	0.6573
20	1.4300	0.7483
21	1.4810	0.7455
22	1.5330	0.7510
23	1.5840	0.6581
24	1.6350	0.4568
25	1.6860	0.1993
26	1.7380	0.0302
27	1.7890	0.0000
28	1.8400	0.0000
29	1.8910	0.0000
30	1.9430	0.0000
31	1.9940	0.0000
32	2.0450	0.0000
33	2.0960	0.0000
34	2.1480	0.0000
35	2.1990	0.0000
36	2.2500	0.0000
37	2.3010	0.0000
38	2.3530	0.0000

39	2.4040	0.0000
40	2.4550	0.0000

ITERATION	SSQ	PECLET	RF
0	2.5125510	5.00000	1.00000
1	2.0375895	6.02197	1.63007
2	1.8661717	16.81586	1.14096
3	1.3585833	28.57618	1.46650
4	1.2421442	55.70067	1.18348
5	0.6307918	77.18728	1.37174
6	0.3239347	132.13273	1.28056
7	0.1571142	206.50526	1.32136
8	0.1274750	264.84063	1.31176
9	0.1242359	294.52444	1.31329
10	0.1240597	302.77202	1.31336
11	0.1240537	304.56661	1.31339
12	0.1240537	304.74452	1.31339
13	0.1240537	304.75780	1.31339

1 CORRELATION MATRIX

	1	2
1	1.0000	
2	0.0775	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	PECLET	304.75780	39.7658	7.66	224.2514	385.2642
2	RF	1.31339	0.0059	220.81	1.3014	1.3254

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.456	0.000	0.000	0.000	1	0.456	0.000	0.000	0.000
2	0.508	0.000	0.000	0.000	2	0.508	0.000	0.000	0.000
3	0.559	0.000	0.000	0.000	3	0.559	0.000	0.000	0.000
4	0.610	0.000	0.000	0.000	4	0.610	0.000	0.000	0.000
5	0.661	0.000	0.000	0.000	5	0.661	0.000	0.000	0.000
6	0.713	0.000	0.000	0.000	6	0.713	0.000	0.000	0.000
7	0.764	0.000	0.000	0.000	7	0.764	0.000	0.000	0.000
8	0.815	0.000	0.000	0.000	40	2.455	0.000	0.000	0.000
9	0.866	0.000	0.000	0.000	8	0.815	0.000	0.000	0.000
10	0.918	0.000	0.000	0.000	39	2.404	0.000	0.000	0.000
11	0.969	0.000	0.000	0.000	38	2.353	0.000	0.000	0.000
12	1.020	0.000	0.001	-0.001	9	0.866	0.000	0.000	0.000
13	1.071	0.002	0.006	-0.003	37	2.301	0.000	0.000	0.000
14	1.123	0.011	0.026	-0.015	36	2.250	0.000	0.000	0.000
15	1.174	0.032	0.083	-0.051	10	0.918	0.000	0.000	0.000
16	1.225	0.093	0.194	-0.102	35	2.199	0.000	0.000	0.000
17	1.276	0.245	0.360	-0.116	34	2.148	0.000	0.000	0.000
18	1.328	0.472	0.554	-0.082	11	0.969	0.000	0.000	0.000
19	1.379	0.657	0.724	-0.066	33	2.096	0.000	0.000	0.000
20	1.430	0.748	0.838	-0.090	32	2.045	0.000	0.000	0.000
21	1.481	0.746	0.875	-0.130	12	1.020	0.000	0.001	-0.001

22	1.533	0.751	0.824	-0.073	31	1.994	0.000	0.002	-0.002
23	1.584	0.658	0.693	-0.035	13	1.071	0.002	0.006	-0.003
24	1.635	0.457	0.513	-0.056	30	1.943	0.000	0.005	-0.005
25	1.686	0.199	0.332	-0.133	29	1.891	0.000	0.015	-0.015
26	1.738	0.030	0.185	-0.155	14	1.123	0.011	0.026	-0.015
27	1.789	0.000	0.091	-0.091	23	1.584	0.658	0.693	-0.035
28	1.840	0.000	0.039	-0.039	28	1.840	0.000	0.039	-0.039
29	1.891	0.000	0.015	-0.015	15	1.174	0.032	0.083	-0.051
30	1.943	0.000	0.005	-0.005	24	1.635	0.457	0.513	-0.056
31	1.994	0.000	0.002	-0.002	19	1.379	0.657	0.724	-0.066
32	2.045	0.000	0.000	0.000	22	1.533	0.751	0.824	-0.073
33	2.096	0.000	0.000	0.000	18	1.328	0.472	0.554	-0.082
34	2.148	0.000	0.000	0.000	20	1.430	0.748	0.838	-0.090
35	2.199	0.000	0.000	0.000	27	1.789	0.000	0.091	-0.091
36	2.250	0.000	0.000	0.000	16	1.225	0.093	0.194	-0.102
37	2.301	0.000	0.000	0.000	17	1.276	0.245	0.360	-0.116
38	2.353	0.000	0.000	0.000	21	1.481	0.746	0.875	-0.130
39	2.404	0.000	0.000	0.000	25	1.686	0.199	0.332	-0.133
40	2.455	0.000	0.000	0.000	26	1.738	0.030	0.185	-0.155

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 10% Methanol/90% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	5.000
2	RF	1.000
3	PUL	0.328

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.3940	0.0000
2	0.4450	0.0000
3	0.4960	0.0000
4	0.5480	0.0000
5	0.5990	0.0000
6	0.6500	0.0000
7	0.7010	0.0000
8	0.7530	0.0000
9	0.8040	0.0000
10	0.8550	0.0000
11	0.9060	0.0000
12	0.9580	0.0000
13	1.0090	0.0000
14	1.0600	0.0018
15	1.1110	0.0041
16	1.1630	0.0353
17	1.2140	0.1728
18	1.2650	0.4012
19	1.3160	0.6129
20	1.3680	0.7223
21	1.4190	0.8058
22	1.4700	0.7435
23	1.5210	0.6161
24	1.5730	0.5071
25	1.6240	0.3088
26	1.6750	0.0880
27	1.7260	0.0000
28	1.7780	0.0000
29	1.8290	0.0000
30	1.8800	0.0000
31	1.9310	0.0000
32	1.9830	0.0000
33	2.0340	0.0000
34	2.0850	0.0000
35	2.1360	0.0000
36	2.1880	0.0000
37	2.2390	0.0000
38	2.2900	0.0000

39	2.3410	0.0000
40	2.3930	0.0000

ITERATION	SSQ	PECLET	RF
0	2.3998257	5.00000	1.00000
1	1.9379348	6.79970	1.57860
2	1.8858709	17.65172	1.07969
3	1.3257426	25.74722	1.40975
4	1.1300019	52.26530	1.15333
5	0.5767929	80.24640	1.32332
6	0.2952515	129.93195	1.23941
7	0.1622297	199.68445	1.27236
8	0.1413681	247.17486	1.26468
9	0.1394053	269.29171	1.26545
10	0.1393203	274.57353	1.26543
11	0.1393184	275.58952	1.26542
12	0.1393184	275.61210	1.26542

1 CORRELATION MATRIX

	1	2
1	1.0000	
2	0.0764	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	PECLET	275.61210	37.8166	7.29	199.0518	352.1724
2	RF	1.26542	0.0064	199.14	1.2526	1.2783

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.394	0.000	0.000	0.000	1	0.394	0.000	0.000	0.000
2	0.445	0.000	0.000	0.000	2	0.445	0.000	0.000	0.000
3	0.496	0.000	0.000	0.000	3	0.496	0.000	0.000	0.000
4	0.548	0.000	0.000	0.000	4	0.548	0.000	0.000	0.000
5	0.599	0.000	0.000	0.000	5	0.599	0.000	0.000	0.000
6	0.650	0.000	0.000	0.000	6	0.650	0.000	0.000	0.000
7	0.701	0.000	0.000	0.000	7	0.701	0.000	0.000	0.000
8	0.753	0.000	0.000	0.000	8	0.753	0.000	0.000	0.000
9	0.804	0.000	0.000	0.000	40	2.393	0.000	0.000	0.000
10	0.855	0.000	0.000	0.000	39	2.341	0.000	0.000	0.000
11	0.906	0.000	0.000	0.000	9	0.804	0.000	0.000	0.000
12	0.958	0.000	0.001	-0.001	38	2.290	0.000	0.000	0.000
13	1.009	0.000	0.004	-0.004	37	2.239	0.000	0.000	0.000
14	1.060	0.002	0.018	-0.017	10	0.855	0.000	0.000	0.000
15	1.111	0.004	0.063	-0.059	36	2.188	0.000	0.000	0.000
16	1.163	0.035	0.160	-0.125	35	2.136	0.000	0.000	0.000
17	1.214	0.173	0.313	-0.140	11	0.906	0.000	0.000	0.000
18	1.265	0.401	0.498	-0.097	34	2.085	0.000	0.000	0.000
19	1.316	0.613	0.676	-0.063	33	2.034	0.000	0.000	0.000
20	1.368	0.722	0.810	-0.088	12	0.958	0.000	0.001	-0.001
21	1.419	0.806	0.871	-0.065	32	1.983	0.000	0.001	-0.001
22	1.470	0.744	0.848	-0.104	31	1.931	0.000	0.003	-0.003

23	1.521	0.616	0.741	-0.125	13	1.009	0.000	0.004	-0.004
24	1.573	0.507	0.571	-0.064	30	1.880	0.000	0.008	-0.008
25	1.624	0.309	0.388	-0.079	14	1.060	0.002	0.018	-0.017
26	1.675	0.088	0.231	-0.143	29	1.829	0.000	0.022	-0.022
27	1.726	0.000	0.120	-0.120	28	1.778	0.000	0.055	-0.055
28	1.778	0.000	0.055	-0.055	15	1.111	0.004	0.063	-0.059
29	1.829	0.000	0.022	-0.022	19	1.316	0.613	0.676	-0.063
30	1.880	0.000	0.008	-0.008	24	1.573	0.507	0.571	-0.064
31	1.931	0.000	0.003	-0.003	21	1.419	0.806	0.871	-0.065
32	1.983	0.000	0.001	-0.001	25	1.624	0.309	0.388	-0.079
33	2.034	0.000	0.000	0.000	20	1.368	0.722	0.810	-0.088
34	2.085	0.000	0.000	0.000	18	1.265	0.401	0.498	-0.097
35	2.136	0.000	0.000	0.000	22	1.470	0.744	0.848	-0.104
36	2.188	0.000	0.000	0.000	27	1.726	0.000	0.120	-0.120
37	2.239	0.000	0.000	0.000	23	1.521	0.616	0.741	-0.125
38	2.290	0.000	0.000	0.000	16	1.163	0.035	0.160	-0.125
39	2.341	0.000	0.000	0.000	17	1.214	0.173	0.313	-0.140
40	2.393	0.000	0.000	0.000	26	1.675	0.088	0.231	-0.143

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 20% Methanol/80% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	5.000
2	RF	1.000
3	PUL	0.322

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4400	0.0000
2	0.4910	0.0000
3	0.5420	0.0000
4	0.5930	0.0000
5	0.6450	0.0000
6	0.6960	0.0000
7	0.7470	0.0000
8	0.7980	0.0000
9	0.8500	0.0000
10	0.9010	0.0000
11	0.9520	0.0000
12	1.0030	0.0000
13	1.0550	0.0017
14	1.1060	0.0017
15	1.1570	0.0043
16	1.2080	0.0173
17	1.2600	0.0605
18	1.3110	0.1710
19	1.3620	0.3301
20	1.4130	0.5278
21	1.4650	0.7038
22	1.5160	0.7881
23	1.5670	0.8223
24	1.6180	0.7540
25	1.6700	0.7254
26	1.7210	0.5936
27	1.7720	0.4118
28	1.8230	0.1756
29	1.8750	0.0421
30	1.9260	0.0000
31	1.9770	0.0000
32	2.0280	0.0000
33	2.0800	0.0000
34	2.1310	0.0000
35	2.1820	0.0000
36	2.2330	0.0000
37	2.2850	0.0000
38	2.3360	0.0000

39	2.3870	0.0000
40	2.4380	0.0000

ITERATION	SSQ	PECLET	RF
0	3.1821863	5.00000	1.00000
1	2.6683041	4.62117	1.76768
2	2.1786787	11.35423	1.40497
3	1.2182719	37.32405	1.44531
4	0.4977078	103.62416	1.35778
5	0.1255254	198.04523	1.43351
6	0.0311304	282.26962	1.40335
7	0.0222684	323.83838	1.41066
8	0.0222296	328.22786	1.41062
9	0.0222295	328.24006	1.41065

1 CORRELATION MATRIX

	1	2
1	1.0000	
2	0.0764	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	PECLET	328.24006	17.6087	18.64	292.5910	363.8891
2	RF	1.41065	0.0026	543.86	1.4054	1.4159

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.440	0.000	0.000	0.000	26	1.721	0.594	0.537	0.057
2	0.491	0.000	0.000	0.000	27	1.772	0.412	0.360	0.051
3	0.542	0.000	0.000	0.000	21	1.465	0.704	0.683	0.021
4	0.593	0.000	0.000	0.000	25	1.670	0.725	0.705	0.020
5	0.645	0.000	0.000	0.000	20	1.413	0.528	0.508	0.020
6	0.696	0.000	0.000	0.000	19	1.362	0.330	0.326	0.004
7	0.747	0.000	0.000	0.000	13	1.055	0.002	0.000	0.002
8	0.798	0.000	0.000	0.000	14	1.106	0.002	0.001	0.001
9	0.850	0.000	0.000	0.000	1	0.440	0.000	0.000	0.000
10	0.901	0.000	0.000	0.000	2	0.491	0.000	0.000	0.000
11	0.952	0.000	0.000	0.000	3	0.542	0.000	0.000	0.000
12	1.003	0.000	0.000	0.000	4	0.593	0.000	0.000	0.000
13	1.055	0.002	0.000	0.002	5	0.645	0.000	0.000	0.000
14	1.106	0.002	0.001	0.001	6	0.696	0.000	0.000	0.000
15	1.157	0.004	0.005	-0.001	7	0.747	0.000	0.000	0.000
16	1.208	0.017	0.023	-0.006	8	0.798	0.000	0.000	0.000
17	1.260	0.060	0.074	-0.013	9	0.850	0.000	0.000	0.000
18	1.311	0.171	0.174	-0.003	10	0.901	0.000	0.000	0.000
19	1.362	0.330	0.326	0.004	40	2.438	0.000	0.000	0.000
20	1.413	0.528	0.508	0.020	11	0.952	0.000	0.000	0.000
21	1.465	0.704	0.683	0.021	39	2.387	0.000	0.000	0.000
22	1.516	0.788	0.806	-0.018	38	2.336	0.000	0.000	0.000
23	1.567	0.822	0.857	-0.035	12	1.003	0.000	0.000	0.000
24	1.618	0.754	0.823	-0.069	37	2.285	0.000	0.000	0.000
25	1.670	0.725	0.705	0.020	36	2.233	0.000	0.000	0.000

26	1.721	0.594	0.537	0.057	35	2.182	0.000	0.000	0.000
27	1.772	0.412	0.360	0.051	34	2.131	0.000	0.001	-0.001
28	1.823	0.176	0.212	-0.037	15	1.157	0.004	0.005	-0.001
29	1.875	0.042	0.109	-0.066	33	2.080	0.000	0.002	-0.002
30	1.926	0.000	0.050	-0.050	18	1.311	0.171	0.174	-0.003
31	1.977	0.000	0.020	-0.020	16	1.208	0.017	0.023	-0.006
32	2.028	0.000	0.007	-0.007	32	2.028	0.000	0.007	-0.007
33	2.080	0.000	0.002	-0.002	17	1.260	0.060	0.074	-0.013
34	2.131	0.000	0.001	-0.001	22	1.516	0.788	0.806	-0.018
35	2.182	0.000	0.000	0.000	31	1.977	0.000	0.020	-0.020
36	2.233	0.000	0.000	0.000	23	1.567	0.822	0.857	-0.035
37	2.285	0.000	0.000	0.000	28	1.823	0.176	0.212	-0.037
38	2.336	0.000	0.000	0.000	30	1.926	0.000	0.050	-0.050
39	2.387	0.000	0.000	0.000	29	1.875	0.042	0.109	-0.066
40	2.438	0.000	0.000	0.000	24	1.618	0.754	0.823	-0.069

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 50% Methanol/50% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	5.000
2	RF	1.000
3	PUL	0.331

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4060	0.0000
2	0.4580	0.0000
3	0.5090	0.0000
4	0.5600	0.0000
5	0.6110	0.0000
6	0.6630	0.0000
7	0.7140	0.0000
8	0.7650	0.0000
9	0.8160	0.0000
10	0.8680	0.0000
11	0.9190	0.0000
12	0.9700	0.0000
13	1.0210	0.0000
14	1.0730	0.0000
15	1.1240	0.0000
16	1.1750	0.0177
17	1.2260	0.0789
18	1.2780	0.2270
19	1.3290	0.3950
20	1.3800	0.6083
21	1.4310	0.7144
22	1.4830	0.7184
23	1.5340	0.7253
24	1.5850	0.7146
25	1.6360	0.6797
26	1.6880	0.5980
27	1.7390	0.4776
28	1.7900	0.2658
29	1.8410	0.0970
30	1.8930	0.0184
31	1.9440	0.0000
32	1.9950	0.0000
33	2.0460	0.0000
34	2.0980	0.0000
35	2.1490	0.0000
36	2.2000	0.0000
37	2.2510	0.0000
38	2.3030	0.0000

39	2.3540	0.0000
40	2.4050	0.0000

ITERATION	SSQ	PECLET	RF
0	2.9583570	5.00000	1.00000
1	2.3833102	5.80803	1.73222
2	1.8883046	13.34307	1.30709
3	1.0679509	39.74408	1.47595
4	0.9037115	91.46498	1.25007
5	0.2358949	114.46765	1.40446
6	0.0712604	182.02134	1.35552
7	0.0467000	218.05743	1.37170
8	0.0465927	221.29075	1.37083
9	0.0465926	221.15155	1.37086
10	0.0465926	221.15960	1.37086

1 CORRELATION MATRIX

	1	2
1	1.0000	
2	0.0615	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	PECLET	221.15960	15.5099	14.26	189.7597	252.5595
2	RF	1.37086	0.0043	319.91	1.3622	1.3795

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.406	0.000	0.000	0.000	27	1.739	0.478	0.383	0.094
2	0.458	0.000	0.000	0.000	20	1.380	0.608	0.525	0.083
3	0.509	0.000	0.000	0.000	26	1.688	0.598	0.529	0.069
4	0.560	0.000	0.000	0.000	21	1.431	0.714	0.664	0.050
5	0.611	0.000	0.000	0.000	19	1.329	0.395	0.371	0.024
6	0.663	0.000	0.000	0.000	25	1.636	0.680	0.667	0.013
7	0.714	0.000	0.000	0.000	28	1.790	0.266	0.253	0.012
8	0.765	0.000	0.000	0.000	1	0.406	0.000	0.000	0.000
9	0.816	0.000	0.000	0.000	2	0.458	0.000	0.000	0.000
10	0.868	0.000	0.000	0.000	3	0.509	0.000	0.000	0.000
11	0.919	0.000	0.000	0.000	4	0.560	0.000	0.000	0.000
12	0.970	0.000	0.000	0.000	5	0.611	0.000	0.000	0.000
13	1.021	0.000	0.001	-0.001	6	0.663	0.000	0.000	0.000
14	1.073	0.000	0.005	-0.005	7	0.714	0.000	0.000	0.000
15	1.124	0.000	0.018	-0.018	8	0.765	0.000	0.000	0.000
16	1.175	0.018	0.052	-0.034	9	0.816	0.000	0.000	0.000
17	1.226	0.079	0.119	-0.041	10	0.868	0.000	0.000	0.000
18	1.278	0.227	0.230	-0.003	40	2.405	0.000	0.000	0.000
19	1.329	0.395	0.371	0.024	11	0.919	0.000	0.000	0.000
20	1.380	0.608	0.525	0.083	39	2.354	0.000	0.000	0.000
21	1.431	0.714	0.664	0.050	38	2.303	0.000	0.000	0.000
22	1.483	0.718	0.763	-0.045	12	0.970	0.000	0.000	0.000
23	1.534	0.725	0.798	-0.073	37	2.251	0.000	0.000	0.000
24	1.585	0.715	0.763	-0.049	36	2.200	0.000	0.001	-0.001

25	1.636	0.680	0.667	0.013	13	1.021	0.000	0.001	-0.001
26	1.688	0.598	0.529	0.069	35	2.149	0.000	0.001	-0.001
27	1.739	0.478	0.383	0.094	18	1.278	0.227	0.230	-0.003
28	1.790	0.266	0.253	0.012	34	2.098	0.000	0.004	-0.004
29	1.841	0.097	0.153	-0.056	14	1.073	0.000	0.005	-0.005
30	1.893	0.018	0.084	-0.066	33	2.046	0.000	0.009	-0.009
31	1.944	0.000	0.043	-0.043	15	1.124	0.000	0.018	-0.018
32	1.995	0.000	0.020	-0.020	32	1.995	0.000	0.020	-0.020
33	2.046	0.000	0.009	-0.009	16	1.175	0.018	0.052	-0.034
34	2.098	0.000	0.004	-0.004	17	1.226	0.079	0.119	-0.041
35	2.149	0.000	0.001	-0.001	31	1.944	0.000	0.043	-0.043
36	2.200	0.000	0.001	-0.001	22	1.483	0.718	0.763	-0.045
37	2.251	0.000	0.000	0.000	24	1.585	0.715	0.763	-0.049
38	2.303	0.000	0.000	0.000	29	1.841	0.097	0.153	-0.056
39	2.354	0.000	0.000	0.000	30	1.893	0.018	0.084	-0.066
40	2.405	0.000	0.000	0.000	23	1.534	0.725	0.798	-0.073

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 0% Methanol/100% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	159.000
2	RF	1.000
3	PUL	0.334

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.5520	0.0000
2	0.6030	0.0000
3	0.6550	0.0000
4	0.7060	0.0000
5	0.7570	0.0000
6	0.8080	0.0000
7	0.8600	0.0000
8	0.9110	0.0000
9	0.9620	0.0005
10	1.0130	0.0021
11	1.0650	0.0084
12	1.1160	0.0597
13	1.1670	0.2889
14	1.2180	0.5989
15	1.2700	0.8106
16	1.3210	0.9129
17	1.3720	0.9490
18	1.4230	0.9235
19	1.4750	0.7407
20	1.5260	0.4700
21	1.5770	0.2397
22	1.6280	0.1175
23	1.6800	0.0521
24	1.7310	0.0261
25	1.7820	0.0160
26	1.8330	0.0123
27	1.8850	0.0103
28	1.9360	0.0089
29	1.9870	0.0078
30	2.0380	0.0067
31	2.0900	0.0058
32	2.1410	0.0048
33	2.1920	0.0036
34	2.2430	0.0028
35	2.2950	0.0022
36	2.3460	0.0017
37	2.3970	0.0013
38	2.4480	0.0011

39	2.5000 0.0010
40	2.5510 0.0008

ITERATION	SSQ	RF
0	3.5356415	1.00000
1	0.3227643	1.16641
2	0.2397820	1.20674
3	0.2355492	1.19223
4	0.2327444	1.19765
5	0.2327444	1.19765

1 CORRELATION MATRIX

	1
1	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	RF	1.19765	0.0097	124.03	1.1781	1.2172

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.552	0.000	0.000	0.000	18	1.423	0.923	0.741	0.182
2	0.603	0.000	0.000	0.000	17	1.372	0.949	0.788	0.161
3	0.655	0.000	0.000	0.000	16	1.321	0.913	0.768	0.145
4	0.706	0.000	0.000	0.000	15	1.270	0.811	0.686	0.124
5	0.757	0.000	0.000	0.000	19	1.475	0.741	0.637	0.104
6	0.808	0.000	0.000	0.000	14	1.218	0.599	0.557	0.042
7	0.860	0.000	0.001	-0.001	30	2.038	0.007	0.001	0.006
8	0.911	0.000	0.007	-0.007	29	1.987	0.008	0.002	0.006
9	0.962	0.001	0.025	-0.024	31	2.090	0.006	0.000	0.006
10	1.013	0.002	0.067	-0.065	32	2.141	0.005	0.000	0.005
11	1.065	0.008	0.147	-0.138	28	1.936	0.009	0.005	0.004
12	1.116	0.060	0.264	-0.204	33	2.192	0.004	0.000	0.004
13	1.167	0.289	0.408	-0.119	34	2.243	0.003	0.000	0.003
14	1.218	0.599	0.557	0.042	35	2.295	0.002	0.000	0.002
15	1.270	0.811	0.686	0.124	36	2.346	0.002	0.000	0.002
16	1.321	0.913	0.768	0.145	37	2.397	0.001	0.000	0.001
17	1.372	0.949	0.788	0.161	38	2.448	0.001	0.000	0.001
18	1.423	0.923	0.741	0.182	39	2.500	0.001	0.000	0.001
19	1.475	0.741	0.637	0.104	40	2.551	0.001	0.000	0.001
20	1.526	0.470	0.502	-0.032	27	1.885	0.010	0.010	0.000
21	1.577	0.240	0.363	-0.123	1	0.552	0.000	0.000	0.000
22	1.628	0.117	0.242	-0.124	2	0.603	0.000	0.000	0.000
23	1.680	0.052	0.147	-0.095	3	0.655	0.000	0.000	0.000
24	1.731	0.026	0.084	-0.058	4	0.706	0.000	0.000	0.000
25	1.782	0.016	0.044	-0.028	5	0.757	0.000	0.000	0.000
26	1.833	0.012	0.022	-0.010	6	0.808	0.000	0.000	0.000
27	1.885	0.010	0.010	0.000	7	0.860	0.000	0.001	-0.001
28	1.936	0.009	0.005	0.004	8	0.911	0.000	0.007	-0.007
29	1.987	0.008	0.002	0.006	26	1.833	0.012	0.022	-0.010
30	2.038	0.007	0.001	0.006	9	0.962	0.001	0.025	-0.024
31	2.090	0.006	0.000	0.006	25	1.782	0.016	0.044	-0.028

32	2.141	0.005	0.000	0.005	20	1.526	0.470	0.502	-0.032
33	2.192	0.004	0.000	0.004	24	1.731	0.026	0.084	-0.058
34	2.243	0.003	0.000	0.003	10	1.013	0.002	0.067	-0.065
35	2.295	0.002	0.000	0.002	23	1.680	0.052	0.147	-0.095
36	2.346	0.002	0.000	0.002	13	1.167	0.289	0.408	-0.119
37	2.397	0.001	0.000	0.001	21	1.577	0.240	0.363	-0.123
38	2.448	0.001	0.000	0.001	22	1.628	0.117	0.242	-0.124
39	2.500	0.001	0.000	0.001	11	1.065	0.008	0.147	-0.138
40	2.551	0.001	0.000	0.001	12	1.116	0.060	0.264	-0.204

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 1% Methanol/99% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	153.000
2	RF	1.000
3	PUL	0.337

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.5040	0.0000
2	0.5550	0.0001
3	0.6070	0.0005
4	0.6580	0.0013
5	0.7090	0.0028
6	0.7600	0.0057
7	0.8120	0.0099
8	0.8630	0.0165
9	0.9140	0.0247
10	0.9650	0.0359
11	1.0170	0.0530
12	1.0680	0.0820
13	1.1190	0.1413
14	1.1700	0.2641
15	1.2220	0.4469
16	1.2730	0.6510
17	1.3240	0.8571
18	1.3750	0.8900
19	1.4270	0.8853
20	1.4780	0.7760
21	1.5290	0.6292
22	1.5800	0.4164
23	1.6320	0.2006
24	1.6830	0.0725
25	1.7340	0.0227
26	1.7850	0.0105
27	1.8370	0.0073
28	1.8880	0.0059
29	1.9390	0.0052
30	1.9900	0.0050
31	2.0420	0.0048
32	2.0930	0.0047
33	2.1440	0.0048
34	2.1950	0.0050
35	2.2470	0.0049
36	2.2980	0.0048
37	2.3490	0.0042
38	2.4000	0.0038

39	2.4520	0.0034
40	2.5030	0.0031

ITERATION	SSQ	RF
0	3.5295768	1.00000
1	0.4832896	1.15290
2	0.1273274	1.23162
3	0.1200646	1.21627
4	0.1184520	1.22041
5	0.1184520	1.22041

1 CORRELATION MATRIX

	1
1	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	RF	1.22041	0.0071	171.67	1.2060	1.2348

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	RESI- OBS.	FITTED	DUAL	PORE NO	CONCENTRATION VOLUME	RESI- OBS.	FITTED	DUAL
1	0.504	0.000	0.000	0.000	19	1.427	0.885	0.755	0.131
2	0.555	0.000	0.000	0.000	17	1.324	0.857	0.732	0.125
3	0.607	0.001	0.000	0.000	18	1.375	0.890	0.775	0.115
4	0.658	0.001	0.000	0.001	20	1.478	0.776	0.676	0.100
5	0.709	0.003	0.000	0.003	21	1.529	0.629	0.558	0.071
6	0.760	0.006	0.000	0.006	9	0.914	0.025	0.005	0.019
7	0.812	0.010	0.000	0.010	16	1.273	0.651	0.634	0.017
8	0.863	0.017	0.001	0.015	10	0.965	0.036	0.019	0.016
9	0.914	0.025	0.005	0.019	8	0.863	0.017	0.001	0.015
10	0.965	0.036	0.019	0.016	7	0.812	0.010	0.000	0.010
11	1.017	0.053	0.055	-0.002	6	0.760	0.006	0.000	0.006
12	1.068	0.082	0.121	-0.039	34	2.195	0.005	0.000	0.005
13	1.119	0.141	0.223	-0.082	35	2.247	0.005	0.000	0.005
14	1.170	0.264	0.355	-0.091	36	2.298	0.005	0.000	0.005
15	1.222	0.447	0.502	-0.055	33	2.144	0.005	0.000	0.005
16	1.273	0.651	0.634	0.017	37	2.349	0.004	0.000	0.004
17	1.324	0.857	0.732	0.125	32	2.093	0.005	0.001	0.004
18	1.375	0.890	0.775	0.115	38	2.400	0.004	0.000	0.004
19	1.427	0.885	0.755	0.131	39	2.452	0.003	0.000	0.003
20	1.478	0.776	0.676	0.100	31	2.042	0.005	0.002	0.003
21	1.529	0.629	0.558	0.071	40	2.503	0.003	0.000	0.003
22	1.580	0.416	0.425	-0.008	5	0.709	0.003	0.000	0.003
23	1.632	0.201	0.296	-0.096	4	0.658	0.001	0.000	0.001
24	1.683	0.072	0.193	-0.120	30	1.990	0.005	0.004	0.001
25	1.734	0.023	0.117	-0.094	3	0.607	0.001	0.000	0.000
26	1.785	0.011	0.066	-0.056	2	0.555	0.000	0.000	0.000
27	1.837	0.007	0.035	-0.027	1	0.504	0.000	0.000	0.000
28	1.888	0.006	0.017	-0.012	11	1.017	0.053	0.055	-0.002
29	1.939	0.005	0.008	-0.003	29	1.939	0.005	0.008	-0.003
30	1.990	0.005	0.004	0.001	22	1.580	0.416	0.425	-0.008
31	2.042	0.005	0.002	0.003	28	1.888	0.006	0.017	-0.012

32	2.093	0.005	0.001	0.004	27	1.837	0.007	0.035	-0.027
33	2.144	0.005	0.000	0.005	12	1.068	0.082	0.121	-0.039
34	2.195	0.005	0.000	0.005	15	1.222	0.447	0.502	-0.055
35	2.247	0.005	0.000	0.005	26	1.785	0.011	0.066	-0.056
36	2.298	0.005	0.000	0.005	13	1.119	0.141	0.223	-0.082
37	2.349	0.004	0.000	0.004	14	1.170	0.264	0.355	-0.091
38	2.400	0.004	0.000	0.004	25	1.734	0.023	0.117	-0.094
39	2.452	0.003	0.000	0.003	23	1.632	0.201	0.296	-0.096
40	2.503	0.003	0.000	0.003	24	1.683	0.072	0.193	-0.120

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 5% Methanol/95% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	305.000
2	RF	1.000
3	PUL	0.309

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.6060	0.0003
2	0.6580	0.0007
3	0.7090	0.0019
4	0.7600	0.0041
5	0.8110	0.0077
6	0.8630	0.0133
7	0.9140	0.0218
8	0.9650	0.0338
9	1.0160	0.0499
10	1.0680	0.0785
11	1.1190	0.1387
12	1.1700	0.2247
13	1.2210	0.3449
14	1.2730	0.5036
15	1.3240	0.7017
16	1.3750	0.8171
17	1.4260	0.8316
18	1.4780	0.7858
19	1.5290	0.6491
20	1.5800	0.3957
21	1.6310	0.1656
22	1.6830	0.0522
23	1.7340	0.0200
24	1.7850	0.0109
25	1.8360	0.0070
26	1.8880	0.0055
27	1.9390	0.0047
28	1.9900	0.0041
29	2.0410	0.0038
30	2.0930	0.0036
31	2.1440	0.0034
32	2.1950	0.0032
33	2.2460	0.0031
34	2.2980	0.0029
35	2.3490	0.0028
36	2.4000	0.0027
37	2.4510	0.0026
38	2.5030	0.0027

39	2.5540	0.0025
40	2.6050	0.0023

ITERATION	SSQ	RF
0	4.4736667	1.00000
1	2.1920920	1.09357
2	0.3298729	1.19663
3	0.0400964	1.24727
4	0.0381951	1.25170
5	0.0381951	1.25171

1 CORRELATION MATRIX

	1
1	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	RF	1.25171	0.0032	394.36	1.2453	1.2581

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.606	0.000	0.000	0.000	11	1.119	0.139	0.083	0.056
2	0.658	0.001	0.000	0.001	10	1.068	0.079	0.025	0.054
3	0.709	0.002	0.000	0.002	9	1.016	0.050	0.005	0.045
4	0.760	0.004	0.000	0.004	8	0.965	0.034	0.001	0.033
5	0.811	0.008	0.000	0.008	19	1.529	0.649	0.618	0.031
6	0.863	0.013	0.000	0.013	12	1.170	0.225	0.202	0.023
7	0.914	0.022	0.000	0.022	7	0.914	0.022	0.000	0.022
8	0.965	0.034	0.001	0.033	6	0.863	0.013	0.000	0.013
9	1.016	0.050	0.005	0.045	5	0.811	0.008	0.000	0.008
10	1.068	0.079	0.025	0.054	18	1.478	0.786	0.781	0.004
11	1.119	0.139	0.083	0.056	27	1.939	0.005	0.001	0.004
12	1.170	0.225	0.202	0.023	4	0.760	0.004	0.000	0.004
13	1.221	0.345	0.379	-0.034	28	1.990	0.004	0.000	0.004
14	1.273	0.504	0.582	-0.078	29	2.041	0.004	0.000	0.004
15	1.324	0.702	0.752	-0.050	30	2.093	0.004	0.000	0.004
16	1.375	0.817	0.854	-0.037	26	1.888	0.005	0.002	0.004
17	1.426	0.832	0.867	-0.036	31	2.144	0.003	0.000	0.003
18	1.478	0.786	0.781	0.004	32	2.195	0.003	0.000	0.003
19	1.529	0.649	0.618	0.031	33	2.246	0.003	0.000	0.003
20	1.580	0.396	0.423	-0.027	34	2.298	0.003	0.000	0.003
21	1.631	0.166	0.249	-0.084	35	2.349	0.003	0.000	0.003
22	1.683	0.052	0.124	-0.072	38	2.503	0.003	0.000	0.003
23	1.734	0.020	0.054	-0.034	36	2.400	0.003	0.000	0.003
24	1.785	0.011	0.021	-0.010	37	2.451	0.003	0.000	0.003
25	1.836	0.007	0.007	0.000	39	2.554	0.003	0.000	0.002
26	1.888	0.005	0.002	0.004	40	2.605	0.002	0.000	0.002
27	1.939	0.005	0.001	0.004	3	0.709	0.002	0.000	0.002
28	1.990	0.004	0.000	0.004	2	0.658	0.001	0.000	0.001
29	2.041	0.004	0.000	0.004	1	0.606	0.000	0.000	0.000
30	2.093	0.004	0.000	0.004	25	1.836	0.007	0.007	0.000
31	2.144	0.003	0.000	0.003	24	1.785	0.011	0.021	-0.010

32	2.195	0.003	0.000	0.003	20	1.580	0.396	0.423	-0.027
33	2.246	0.003	0.000	0.003	23	1.734	0.020	0.054	-0.034
34	2.298	0.003	0.000	0.003	13	1.221	0.345	0.379	-0.034
35	2.349	0.003	0.000	0.003	17	1.426	0.832	0.867	-0.036
36	2.400	0.003	0.000	0.003	16	1.375	0.817	0.854	-0.037
37	2.451	0.003	0.000	0.003	15	1.324	0.702	0.752	-0.050
38	2.503	0.003	0.000	0.003	22	1.683	0.052	0.124	-0.072
39	2.554	0.003	0.000	0.002	14	1.273	0.504	0.582	-0.078
40	2.605	0.002	0.000	0.002	21	1.631	0.166	0.249	-0.084

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 10% Methanol/90% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	276.000
2	RF	1.000
3	PUL	0.320

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4500	0.0002
2	0.5010	0.0007
3	0.5530	0.0018
4	0.6040	0.0044
5	0.6550	0.0077
6	0.7060	0.0122
7	0.7580	0.0181
8	0.8090	0.0242
9	0.8600	0.0328
10	0.9110	0.0406
11	0.9630	0.0507
12	1.0140	0.0659
13	1.0650	0.0934
14	1.1160	0.1523
15	1.1680	0.2284
16	1.2190	0.3264
17	1.2700	0.5001
18	1.3210	0.6810
19	1.3730	0.7971
20	1.4240	0.8124
21	1.4750	0.7504
22	1.5260	0.6556
23	1.5780	0.4617
24	1.6290	0.2220
25	1.6800	0.0719
26	1.7310	0.0266
27	1.7830	0.0139
28	1.8340	0.0093
29	1.8850	0.0068
30	1.9360	0.0054
31	1.9880	0.0045
32	2.0390	0.0038
33	2.0900	0.0033
34	2.1410	0.0029
35	2.1930	0.0026
36	2.2440	0.0024
37	2.2950	0.0022
38	2.3460	0.0021

39	2.3980	0.0020
40	2.4490	0.0019

ITERATION	SSQ	RF
0	4.1831929	1.00000
1	1.9238347	1.09672
2	0.2849047	1.19765
3	0.0550446	1.24384
4	0.0528172	1.24887
5	0.0528172	1.24887

1 CORRELATION MATRIX

	1
1	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	RF	1.24887	0.0038	325.63	1.2411	1.2566

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.450	0.000	0.000	0.000	13	1.065	0.093	0.030	0.063
2	0.501	0.001	0.000	0.001	14	1.116	0.152	0.093	0.060
3	0.553	0.002	0.000	0.002	12	1.014	0.066	0.007	0.059
4	0.604	0.004	0.000	0.004	11	0.963	0.051	0.001	0.050
5	0.655	0.008	0.000	0.008	10	0.911	0.041	0.000	0.041
6	0.706	0.012	0.000	0.012	9	0.860	0.033	0.000	0.033
7	0.758	0.018	0.000	0.018	8	0.809	0.024	0.000	0.024
8	0.809	0.024	0.000	0.024	7	0.758	0.018	0.000	0.018
9	0.860	0.033	0.000	0.033	15	1.168	0.228	0.215	0.013
10	0.911	0.041	0.000	0.041	6	0.706	0.012	0.000	0.012
11	0.963	0.051	0.001	0.050	5	0.655	0.008	0.000	0.008
12	1.014	0.066	0.007	0.059	22	1.526	0.656	0.650	0.005
13	1.065	0.093	0.030	0.063	4	0.604	0.004	0.000	0.004
14	1.116	0.152	0.093	0.060	30	1.936	0.005	0.001	0.004
15	1.168	0.228	0.215	0.013	31	1.988	0.004	0.000	0.004
16	1.219	0.326	0.388	-0.061	32	2.039	0.004	0.000	0.004
17	1.270	0.500	0.578	-0.077	33	2.090	0.003	0.000	0.003
18	1.321	0.681	0.741	-0.060	29	1.885	0.007	0.004	0.003
19	1.373	0.797	0.845	-0.048	34	2.141	0.003	0.000	0.003
20	1.424	0.812	0.866	-0.053	35	2.193	0.003	0.000	0.003
21	1.475	0.750	0.796	-0.046	36	2.244	0.002	0.000	0.002
22	1.526	0.656	0.650	0.005	37	2.295	0.002	0.000	0.002
23	1.578	0.462	0.463	-0.001	38	2.346	0.002	0.000	0.002
24	1.629	0.222	0.289	-0.067	39	2.398	0.002	0.000	0.002
25	1.680	0.072	0.158	-0.086	40	2.449	0.002	0.000	0.002
26	1.731	0.027	0.075	-0.049	3	0.553	0.002	0.000	0.002
27	1.783	0.014	0.031	-0.017	2	0.501	0.001	0.000	0.001
28	1.834	0.009	0.012	-0.002	1	0.450	0.000	0.000	0.000
29	1.885	0.007	0.004	0.003	23	1.578	0.462	0.463	-0.001
30	1.936	0.005	0.001	0.004	28	1.834	0.009	0.012	-0.002
31	1.988	0.004	0.000	0.004	27	1.783	0.014	0.031	-0.017

32	2.039	0.004	0.000	0.004	21	1.475	0.750	0.796	-0.046
33	2.090	0.003	0.000	0.003	19	1.373	0.797	0.845	-0.048
34	2.141	0.003	0.000	0.003	26	1.731	0.027	0.075	-0.049
35	2.193	0.003	0.000	0.003	20	1.424	0.812	0.866	-0.053
36	2.244	0.002	0.000	0.002	18	1.321	0.681	0.741	-0.060
37	2.295	0.002	0.000	0.002	16	1.219	0.326	0.388	-0.061
38	2.346	0.002	0.000	0.002	24	1.629	0.222	0.289	-0.067
39	2.398	0.002	0.000	0.002	17	1.270	0.500	0.578	-0.077
40	2.449	0.002	0.000	0.002	25	1.680	0.072	0.158	-0.086

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 20% Methanol/80% Water

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INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	328.000
2	RF	1.000
3	PUL	0.313

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4830	0.0125
2	0.5350	0.0172
3	0.5860	0.0221
4	0.6370	0.0276
5	0.6880	0.0330
6	0.7400	0.0374
7	0.7910	0.0444
8	0.8420	0.0516
9	0.8930	0.0607
10	0.9450	0.0735
11	0.9960	0.0930
12	1.0470	0.1491
13	1.0980	0.2285
14	1.1500	0.3114
15	1.2010	0.3575
16	1.2520	0.4748
17	1.3030	0.6591
18	1.3550	0.8305
19	1.4060	0.8706
20	1.4570	0.7595
21	1.5080	0.6463
22	1.5600	0.4454
23	1.6110	0.2223
24	1.6620	0.0708
25	1.7130	0.0333
26	1.7650	0.0120
27	1.8160	0.0140
28	1.8670	0.0111
29	1.9180	0.0092
30	1.9700	0.0075
31	2.0210	0.0072
32	2.0720	0.0056
33	2.1230	0.0052
34	2.1750	0.0047
35	2.2260	0.0046
36	2.2770	0.0044
37	2.3280	0.0043
38	2.3800	0.0044

39	2.4310	0.0043
40	2.4820	0.0040

ITERATION	SSQ	RF
0	3.7921204	1.00000
1	1.8465650	1.08619
2	0.4169640	1.17352
3	0.1260098	1.22018
4	0.1150433	1.23034
5	0.1150326	1.23175
6	0.1150326	1.23175

1 CORRELATION MATRIX

	1
1	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	RF	1.23175	0.0053	233.02	1.2211	1.2424

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.483	0.013	0.000	0.013	13	1.098	0.229	0.070	0.158
2	0.535	0.017	0.000	0.017	12	1.047	0.149	0.018	0.131
3	0.586	0.022	0.000	0.022	14	1.150	0.311	0.189	0.122
4	0.637	0.028	0.000	0.028	11	0.996	0.093	0.003	0.090
5	0.688	0.033	0.000	0.033	10	0.945	0.073	0.000	0.073
6	0.740	0.037	0.000	0.037	9	0.893	0.061	0.000	0.061
7	0.791	0.044	0.000	0.044	8	0.842	0.052	0.000	0.052
8	0.842	0.052	0.000	0.052	7	0.791	0.044	0.000	0.044
9	0.893	0.061	0.000	0.061	6	0.740	0.037	0.000	0.037
10	0.945	0.073	0.000	0.073	5	0.688	0.033	0.000	0.033
11	0.996	0.093	0.003	0.090	4	0.637	0.028	0.000	0.028
12	1.047	0.149	0.018	0.131	3	0.586	0.022	0.000	0.022
13	1.098	0.229	0.070	0.158	2	0.535	0.017	0.000	0.017
14	1.150	0.311	0.189	0.122	1	0.483	0.013	0.000	0.013
15	1.201	0.357	0.373	-0.015	28	1.867	0.011	0.001	0.010
16	1.252	0.475	0.583	-0.108	22	1.560	0.445	0.436	0.009
17	1.303	0.659	0.762	-0.103	29	1.918	0.009	0.000	0.009
18	1.355	0.831	0.874	-0.043	27	1.816	0.014	0.005	0.009
19	1.406	0.871	0.893	-0.022	30	1.970	0.007	0.000	0.007
20	1.457	0.759	0.813	-0.053	31	2.021	0.007	0.000	0.007
21	1.508	0.646	0.647	0.000	32	2.072	0.006	0.000	0.006
22	1.560	0.445	0.436	0.009	33	2.123	0.005	0.000	0.005
23	1.611	0.222	0.251	-0.028	34	2.175	0.005	0.000	0.005
24	1.662	0.071	0.122	-0.051	35	2.226	0.005	0.000	0.005
25	1.713	0.033	0.050	-0.017	38	2.380	0.004	0.000	0.004
26	1.765	0.012	0.017	-0.005	36	2.277	0.004	0.000	0.004
27	1.816	0.014	0.005	0.009	39	2.431	0.004	0.000	0.004
28	1.867	0.011	0.001	0.010	37	2.328	0.004	0.000	0.004
29	1.918	0.009	0.000	0.009	40	2.482	0.004	0.000	0.004
30	1.970	0.007	0.000	0.007	21	1.508	0.646	0.647	0.000

31	2.021	0.007	0.000	0.007	26	1.765	0.012	0.017	-0.005
32	2.072	0.006	0.000	0.006	15	1.201	0.357	0.373	-0.015
33	2.123	0.005	0.000	0.005	25	1.713	0.033	0.050	-0.017
34	2.175	0.005	0.000	0.005	19	1.406	0.871	0.893	-0.022
35	2.226	0.005	0.000	0.005	23	1.611	0.222	0.251	-0.028
36	2.277	0.004	0.000	0.004	18	1.355	0.831	0.874	-0.043
37	2.328	0.004	0.000	0.004	24	1.662	0.071	0.122	-0.051
38	2.380	0.004	0.000	0.004	20	1.457	0.759	0.813	-0.053
39	2.431	0.004	0.000	0.004	17	1.303	0.659	0.762	-0.103
40	2.482	0.004	0.000	0.004	16	1.252	0.475	0.583	-0.108

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 50% Methanol/50% Water

****

INITIAL VALUES OF COEFFICIENTS

NO	NAME	INITIAL VALUE
1	PECLET	221.000
2	RF	1.000
3	PUL	0.326

OBSERVED DATA

OBS. NO.	PORE VOLUME	CONCENTRATION
1	0.4330	0.0084
2	0.4850	0.0136
3	0.5360	0.0191
4	0.5870	0.0237
5	0.6380	0.0296
6	0.6900	0.0352
7	0.7410	0.0384
8	0.7920	0.0453
9	0.8430	0.0511
10	0.8950	0.0757
11	0.9460	0.0688
12	0.9970	0.0902
13	1.0480	0.1298
14	1.1000	0.2016
15	1.1510	0.2740
16	1.2020	0.3354
17	1.2530	0.4179
18	1.3050	0.5865
19	1.3560	0.8007
20	1.4070	0.9018
21	1.4580	0.8672
22	1.5100	0.7320
23	1.5610	0.4621
24	1.6120	0.2397
25	1.6630	0.1438
26	1.7150	0.0839
27	1.7660	0.0619
28	1.8170	0.0458
29	1.8680	0.0300
30	1.9200	0.0191
31	1.9710	0.0122
32	2.0220	0.0083
33	2.0730	0.0057
34	2.1250	0.0048
35	2.1760	0.0039
36	2.2270	0.0034
37	2.2780	0.0030
38	2.3300	0.0026

39	2.3810	0.0024
40	2.4320	0.0022

ITERATION	SSQ	RF
0	3.8082657	1.00000
1	1.5077115	1.10596
2	0.1944039	1.20882
3	0.1126366	1.23999
4	0.1126193	1.24035

1 CORRELATION MATRIX

	1
1	1.0000

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

VARIABLE	NAME	VALUE	S.E.COEFF.	T-VALUE	95% CONFIDENCE LIMITS LOWER	UPPER
1	RF	1.24035	0.0061	204.98	1.2281	1.2526

-----ORDERED BY COMPUTER INPUT-----					-----ORDERED BY RESIDUALS-----				
PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL	PORE NO	CONCENTRATION VOLUME	OBS.	FITTED	RESI-DUAL
1	0.433	0.008	0.000	0.008	14	1.100	0.202	0.103	0.099
2	0.485	0.014	0.000	0.014	13	1.048	0.130	0.038	0.092
3	0.536	0.019	0.000	0.019	12	0.997	0.090	0.011	0.080
4	0.587	0.024	0.000	0.024	21	1.458	0.867	0.788	0.079
5	0.638	0.030	0.000	0.030	10	0.895	0.076	0.000	0.075
6	0.690	0.035	0.000	0.035	20	1.407	0.902	0.835	0.067
7	0.741	0.038	0.000	0.038	11	0.946	0.069	0.002	0.067
8	0.792	0.045	0.000	0.045	22	1.510	0.732	0.669	0.063
9	0.843	0.051	0.000	0.051	15	1.151	0.274	0.215	0.059
10	0.895	0.076	0.000	0.075	9	0.843	0.051	0.000	0.051
11	0.946	0.069	0.002	0.067	8	0.792	0.045	0.000	0.045
12	0.997	0.090	0.011	0.080	7	0.741	0.038	0.000	0.038
13	1.048	0.130	0.038	0.092	6	0.690	0.035	0.000	0.035
14	1.100	0.202	0.103	0.099	5	0.638	0.030	0.000	0.030
15	1.151	0.274	0.215	0.059	4	0.587	0.024	0.000	0.024
16	1.202	0.335	0.370	-0.035	28	1.817	0.046	0.026	0.020
17	1.253	0.418	0.541	-0.124	29	1.868	0.030	0.011	0.019
18	1.305	0.587	0.698	-0.111	3	0.536	0.019	0.000	0.019
19	1.356	0.801	0.801	-0.001	30	1.920	0.019	0.004	0.015
20	1.407	0.902	0.835	0.067	2	0.485	0.014	0.000	0.014
21	1.458	0.867	0.788	0.079	31	1.971	0.012	0.001	0.011
22	1.510	0.732	0.669	0.063	1	0.433	0.008	0.000	0.008
23	1.561	0.462	0.511	-0.049	32	2.022	0.008	0.000	0.008
24	1.612	0.240	0.349	-0.109	33	2.073	0.006	0.000	0.006
25	1.663	0.144	0.214	-0.070	34	2.125	0.005	0.000	0.005
26	1.715	0.084	0.116	-0.032	27	1.766	0.062	0.058	0.004
27	1.766	0.062	0.058	0.004	35	2.176	0.004	0.000	0.004
28	1.817	0.046	0.026	0.020	36	2.227	0.003	0.000	0.003
29	1.868	0.030	0.011	0.019	37	2.278	0.003	0.000	0.003
30	1.920	0.019	0.004	0.015	38	2.330	0.003	0.000	0.003
31	1.971	0.012	0.001	0.011	39	2.381	0.002	0.000	0.002
32	2.022	0.008	0.000	0.008	40	2.432	0.002	0.000	0.002

33	2.073	0.006	0.000	0.006	19	1.356	0.801	0.801	-0.001
34	2.125	0.005	0.000	0.005	26	1.715	0.084	0.116	-0.032
35	2.176	0.004	0.000	0.004	16	1.202	0.335	0.370	-0.035
36	2.227	0.003	0.000	0.003	23	1.561	0.462	0.511	-0.049
37	2.278	0.003	0.000	0.003	25	1.663	0.144	0.214	-0.070
38	2.330	0.003	0.000	0.003	24	1.612	0.240	0.349	-0.109
39	2.381	0.002	0.000	0.002	18	1.305	0.587	0.698	-0.111
40	2.432	0.002	0.000	0.002	17	1.253	0.418	0.541	-0.124

END OF PROBLEM

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